Forty Bravais lattices of four-dimensional space

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Abstract

The method deriving Bravais lattices, especially non-primitive lattices, is discussed. The principles introduced to derive non-primitive lattices are:

(1) Rotative-translative invariance of the centering vectors for the primitive lattices.

(2) Similarity of the centering vectors.

(3) Closure of centering vectors.

The number of the primitive lattices in four-dimensional space is shown to be 18 and that of non-primitive is done to be 22.

1. Introduction

Burzlaff & Zimmermann (1983) described that "The Bravais lattices may be derived by topological procedures (Delaunay, 1933) or algebraic ones (Burckhardt, 1966; Neubüser, Wondratschek and Bülow, 1971)". Regrettably, there is no description of completed algebraic method of derivation of Bravais lattices even in three-dimensional space in Burckhardt (1966).

There are many investigations on Bravais lattices, but the fact that the number of Bravais lattices in four-dimensional space was not uniquely determined and various numbers of the lattices were proposed by the various investigators indicates the lack of the principles to derive Bravais lattices. Mackey & Pawley (1963) discussed the lattices and concluded that the number of the lattice was 52 (21 primitive and 31 non-primitive). Neubüser & Wondratschek (1969) discussed that the number was 64 (33 primitive and 31 non-primitive). Kuntsevich & Belov (1970) obtained 55 Bravais lattices (26 primitive and 29 non-primitive). We can not see even the definition of Bravais lattices in these articles, although the restrictions for the centering vectors of Mackay and Pawley (1963) and the geometrical method of Burckhardt (1966) approached to near the nature of Bravais lattices. Novertheless, their methods could not reached the decisive determination of the Bravais lattices in general space.

Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978) published the results of their electronic computer study. Hereafter, their results are referred as B. B. N. W. Z. When the present author read their lists, he felt very strange, since two crystal systems shared the same lattice. The present author's understanding for a crystal system is that a crystal system

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consists of crystal classes of which symmetry operations make invariantly transform a lattice into itself. That is to say, a lattice decides the crystal system. Lattice vectors in a conventional unit cell or on the boundary of the cell of non-primitive lattices, centering vectors, are independent of one another for two- and three-dimensional lattices. The centering vectors of four-dimensional space should also be independent of one another. Nevertheless, there are not independent centering vectors in their Bravais lattices. In addition, their bases of the some lattices are not always reduced, since the number 2 appears in their representation matrices. We can not know the method of the derivation of Bravais lattices in their book. The method which the present author supposed to be their method is discussed in the final section in this article.

Bravais lattices in any dimensional space can be obtained if point groups for the space are determined. Four-dimensional point groups were derived by Hurley (1951) depending upon the theory of Goursat (1889). The results were revised by Hurley, Neubüser & Wondratschek (1967). Since there are many crystal systems which seem to be merged to the other crystal systems in the crystal systems of *B. B. N. W. Z.*, their principle to determine crystal systems is not approved. Therefore, their results should be fundamentally examined from the crystallographic point of view. Although the present author's examination on the point groups of four-dimensional space is not completed still, the results of *B. B. N. W. Z.* can be available for the derivation of the Bravais lattices.

A symmetrical property of lattices that lattices are invariant for translation and rotation operations is expressed as the rotative-translative invariance in this article. All the lattice points of a non-primitive lattice can be transformed to have integral coordinates by adapting the fractional bases of the corresponding primitive lattice. There is a subset which is isomorphic to the set of lattice points of the primitive lattice in the set of the non-primitive lattice points. The subset composes of the lattice points of which coordinates are the integral multiples of those of the lattice points of the primitive lattices. Then, the set of the coset representatives of the cosets of the subset in the non-primitive lattice is a subset of the coset representatives of the subset in the primitive lattece, in other words, the set of the lattice points of the non-primitive lattice is a subset of the set of the lattice points of the primitive lattice. The coset representatives become centering vectors when the bases are again transformed to the ordinary ones. The problem to derive non-primitive lattices from a primitive lattice becomes to study the conditions that the sets of the coset representatives, the centering vectors, of the non-primitive lattices should satisfy.

The representations of the symmetry operations belonging to the holohedry of a primitive lattice are invariant for some exchanges of the bases of the lattice, although the bases are not symmetrically equivalent. This kind of the exchanges of the bases is called similar operation in this article. Similar operations are one-to-one mappings of the lattice as a whole, and form a group. The non-primitive lattices derived from a primitive lattices in three-dimensional space can be characterized by the difference of the similar operations and the centering vectors. This similarity of the bases of lattices is adapted as the one of principles to derive non-primitive lattices.

Since derivation of primitive lattices from point group symmetries is very easy by the use of word processors, the present author discusses mainly the method to derive non-primitive lattices in four-dimensional space and shows that the number of Bravais lattices is 40 (18 primitive and 22 non-primitive). The number was suggested by a certain Russian crystallographer.

2. Preliminary Remarks

The terms and the concepts used in this article are explained shortly in this section. The methods and the principles established previously and related with the present author's method are alse described.

2. 1. Lattices and reduced bases

The infinite set of vectors-which are linear combinations of n independent vectors with integral coefficients is called a lattice in n-dimensional space. The starting point of the vectors is fixed and is called the origin of lattice. The n independent vectors are called the bases. The members of the set are called the lattice vectors. The set of the bases is called the basis of the lattice. The origin of the lattice and the end points of the lattice vectors are called lattice points. The lattice is also defined as the set of the lattice points. The integral coefficients of the bases in the lattice vectors are called coordinates of the lattice points. The lattice of n-dimensional space is represented by

$$\boldsymbol{V}_p = \{\sum_i^n p_i \boldsymbol{a}_i; -\infty \leq p_i \leq \infty\}, \tag{2. 1. 1}$$

where $\boldsymbol{a}_i$ is the i th base and p_i is an integer.

A n-dimensional domain of polyhedron of which apexes of 2^n are at lattice points and no lattice point exists in the domain is called a n-dimensional unit cell. Although the every volume of the n-dimensional unit cells of a lattice in n-dimensional space is equal, there are infinite many shapes of unit cells. By fixing an apex as the origin of the unit cell, the vectors from the origin to the remaining apexes can be the bases of the lattice.

The bases are chosen from the above vectors and linear combinations of them. When the bases satisfy the following condition,

$$|\boldsymbol{a}_i + \boldsymbol{a}_j| \geq |\boldsymbol{a}_i| \text{ for } i \neq j, \tag{2. 1. 2}$$

the basis is called to be reduced. There are many possible bases for a lattice, even though the bases are reduced.

Notations of points and vectors are of the same form and expressed by bold italic styles, the representations of the points and the vectors which are given by row (the expression in the text) or column (the practical calculations) matrices are expressed by bold styles in this article.

2. 2. Symmetry operations and their representation

Rigid movements of a lattice which make coincide the lattice with itself are called symmetry operations. When symmetry operations displace the lattice parallel, the symmetry operations are called translation operations. The translation operations of the lattice form a group, and can be represented by the form of equation (2. 1. 1), that is, the translation groups are represented by the same forms with the lattices and are not necessary to distinguish each other. Of course, another form of the representation is possible, see Burckhardt (1966). When the symmetry operations rotate the lattice (in wide sense) by fixing the origin, the symmetry operations are called point group symmetry operations. The point group symmetry operations of the lattice form a point group.

There is the maximum group in the point groups for a lattice. The other point groups of the lattice are the subgroups of the group. The maximum group is called the holohedry of the lattice. There are many possible reduced bases which can span the lattice. Symmetry operations which make one-to-one correspondence of the reduced bases are symmetry operations of the holohedry.

The point group symmetry operations of four-dimensional space given by Mackay & Pawley (1963) are listed in Table 1.

A basis for the representations of symmetry operations is also expressed by a column matrix of which elements are the bases as follows,

$$[\boldsymbol{a}] = \begin{vmatrix} \boldsymbol{a}_1 \\ \boldsymbol{a}_2 \\ \boldsymbol{a}_3 \end{vmatrix}. \qquad (2.\ 2.\ 1)$$

When bases of two lattices are $[\boldsymbol{a}]$ and $[\boldsymbol{b}]$, and the two bases are related by a transformation matrix $\boldsymbol{T}$,

$$[\boldsymbol{b}] = \boldsymbol{T}[\boldsymbol{a}], \qquad (2.\ 2.\ 2)$$

a symmetry operations $\boldsymbol{R}$ represented on the basis $[\boldsymbol{a}]$, which brings $[\boldsymbol{a}]$ to $[\boldsymbol{a}']$ by

$$[\boldsymbol{a}'] = \boldsymbol{R}[\boldsymbol{a}], \qquad (2.\ 2.\ 3)$$

that is,

$$\boldsymbol{a}'_i = \sum_j^n R_{ij}\boldsymbol{a}_j, \qquad (2.\ 2.\ 3')$$

is transformed to $\boldsymbol{R}'$ in case of the basis being $[\boldsymbol{b}]$,

$$\boldsymbol{R}' = \boldsymbol{T}\boldsymbol{R}\boldsymbol{T}^{-1}. \qquad (2.\ 2.\ 4)$$

2. 3. Reduction of quadratic forms and representations of symmetry operations

A quadratic form ϕ is defined by the product of a square matrix $\boldsymbol{A}$, a column vector $\boldsymbol{x}$ of which elements are integers, and the transposed vector $\boldsymbol{x}^t$ as follows,

$$\phi = \boldsymbol{x}^t \boldsymbol{A} \boldsymbol{x}. \tag{2. 3. 1}$$

Without changing the values of quadratic forms, to change the diagonal elements of $\boldsymbol{A}$ to the possibly largest values and the off-diagonal elements to the possibly smallest values is called the reduction of quadratic form.

A lattice is also characterized by the metric tensor. The metric tensor for the basis $[\boldsymbol{a}]$ is expressed by

$$\boldsymbol{M} = [\boldsymbol{a}][\boldsymbol{a}]^t. \tag{2. 3. 2}$$

When the matrix $\boldsymbol{A}$ is substituted by the metric tensor $\boldsymbol{M}$ and the elements of the column vector are coordinates of a lattice point $\boldsymbol{x}$, the quadratic form becomes the square of the lattice vector $\boldsymbol{x}$. Hence, quadratic forms correspond to the squares of lattices vectors. Since there are infinite many choices of the basis of a lattice, there are infinite many quadratic forms for a lattice vector.

Symmetry operations of the point group of a lattice transform invariantly the metric tensor of the lattice. If a metric tensor $\boldsymbol{M}$ is invariant for a rotation $\boldsymbol{R}$, $\boldsymbol{M} = \boldsymbol{R}\boldsymbol{M}\boldsymbol{R}^t$, the metric tensor $\boldsymbol{M}' = [\boldsymbol{b}][\boldsymbol{b}]^t$ is also invariant by $\boldsymbol{R}' = \boldsymbol{T}\boldsymbol{R}\boldsymbol{T}^{-1}$. We can see that if $\boldsymbol{T}$ is a non-singular matrix, then any metric tensor transformed by $\boldsymbol{T}$ is invariant for the symmetry operations of the lattice. We can not use the invariance of metric tensor for the criterion of the existence of a new type of lattice. The matrix $\boldsymbol{M}$ in equation (2. 3. 2) is composed of the basis of a lattice, so that the study of the reduction of quadratic forms seemed to be useful for the study of the nature of Bravais lattices. The reduction is essentially to obtain reduced bases of given lattices, and not related with the derivation of Bravais lattices in itself.

Reduction of quadratic forms was discussed by many authors, the present author refers Minkowski (1883). According to him, a quadratic form is reduced if

$$a_{11} \leq a_{22} \leq \ldots \leq a_{nn} \tag{2. 3. 3}$$

and

$$\phi(\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n) \geq a_{hh}, \tag{2. 3. 4}$$

where a_{ij} is the ij element of $\boldsymbol{A}$, ε_h is 1 and the other ε_k are 0 or ± 1.

There is a very simple relation between equations (2. 2. 3') and (2. 3. 4). When $h = i$ and the both sides of equation (2. 3. 4) are equal, then $a_{hh} = \boldsymbol{a}_i'^2$ and $\varepsilon_j = R_{ij}$. Equation (2. 2. 3') is for the case of $h = i$ and $\varepsilon_k = 0 (j \neq k)$ in equation (2. 3. 4). Hence, the row matrices of which i th element is ε_i must be the h th row of a symmetry operation R. From these relations, it is concluded that symmetry operations represented on the reduced bases have only elements of 0, or $\pm$ 1. Matrices of which determinant are $\pm$ 1 and of which elements are integers are called to be unimodular, but unimodular matrices in this article mean the unimodular matrices with the elements 0 or $\pm$ 1.

2. 4. Rotative-translative invariance of lattices

Two vectors (points) $\boldsymbol{x}$ and $\boldsymbol{x}'$ are called to be translatively equivalent, if the vectors are related with

$$\boldsymbol{x}' = \boldsymbol{x} - (\sum_{i}^{n} c_i \boldsymbol{a}_i), \tag{2. 4. 1}$$

where $\sum_{i}^{n} c_i \boldsymbol{a}_i$ is a lattice vector. All the lattice vectors of a lattice are translatively equivalent to one another. Buckhardt (1966) expressed this relation as follows,

$$\boldsymbol{x}' \equiv \boldsymbol{x}(mod.\ 1). \tag{2. 4. 2}$$

This notation is convenient to express the translative equivalence, the present author uses this notation. A point group symmetry operation $\boldsymbol{R}$ brings a lattice vector $\boldsymbol{x}$ to another lattice vector $\boldsymbol{x}'$. The lattice vector $\boldsymbol{x}'$ should be translatively equivalent to $\boldsymbol{x}$. Therefore, a point group symmetry operation satisfies the following equation,

$$\boldsymbol{R}^t\boldsymbol{x} \equiv \boldsymbol{x}(mod.\ 1). \tag{2. 4. 3}$$

The two vectors $\boldsymbol{x}$ and $\boldsymbol{x}' = \boldsymbol{R}^t\boldsymbol{x}$ satisfying equation (2. 4. 3) are called rotative-translatively equivalent to each other for the lattice. The most important symmetrical property of lattices to derived non-primitive lattices is rotative-translative invariance of the lattices.

3. Nature of Bravais lattices

There is no decisive definition of Bravais lattices until now. In order to give definition of Brarais lattices, their nature is to be studied.

3. 1. Translation groups of non-primitive lattices

The translation group of a primitive lattice is represented by the form of equation (2. 1. 1). Non-primitive lattices have more lattice points in addition to those of the corresponding primitive lattices. The additional lattice points should have translation symmetries of the primitive lattices. That is to say, there are lattice vectors of the primitive lattices in the additions or the subtractions of the additional lattices vectors. The coordinates of these additional lattice points can be transformed to integers by multiplying common integral numbers, if not, the additional lattice points do not have translation symmetries of the primitive lattices.

When the least common multiple making all coordinates of the lattice points of a non-primitive lattice be integers is m, the corresponding primitive lattice can be expressed by a union (a sum in this case) of cosets of $\boldsymbol{V}_P'$, which is a subset of the lattice, in $\boldsymbol{V}_P$ as follows. The elements of $\boldsymbol{V}_P'$ are expressed by the multiples of those of the primitive lattice by m, then equation (2. 1. 1) is rewritten by

$$\boldsymbol{V_P} = \boldsymbol{V_P}' + (\boldsymbol{x}_1 + \boldsymbol{V_P}') + \ldots + (\boldsymbol{x}_q + \boldsymbol{V_P}'). \tag{3. 1. 1}$$

where

$$\boldsymbol{V_P}' = \{\sum_i^n m(p_i \boldsymbol{a}_i); -\infty \leq p_i \leq \infty\},$$

When $m = 2$, then $q = 3$, 7 and 15 for two-, three- and four- dimensional primitive lattices, respectively. The subset $(\boldsymbol{x}_i + \boldsymbol{V_P}')$ is called a (right) coset of $\boldsymbol{V_P}'$ in $\boldsymbol{V_P}$. The vectors $\boldsymbol{x}_i s$ are called the coset representatives of the cosets $(\boldsymbol{x}_i + \boldsymbol{V_P}')s$. By dividing the elements of $\boldsymbol{V_P}$ in equation (3. 1. 1) by m, the coefficient of the vectors $\boldsymbol{x}_i$ become fractional numbers. The vectors $\boldsymbol{x}_i$ with fractional coefficients are rewritten by $\boldsymbol{t}_i$, and called centering vectors. That is, the centering vectors are the coset representatives. The primitive lattice with the fractional coefficients is expressed by the following form,

$$\boldsymbol{V_P}'' = \boldsymbol{V_P} + (\boldsymbol{t}_1 + \boldsymbol{V_P}) + \ldots + (\boldsymbol{t}_q + \boldsymbol{V_P}). \tag{3. 1. 2}$$

It must be noticed that $\boldsymbol{V_P}$ in equation (3. 1. 1) is quite the same form as that in equation (3. 1. 2), that is, the subset $\boldsymbol{V_P}$ in equation (3. 1. 2) is isomorphic to the set $\boldsymbol{V_P}$ and the subset $\boldsymbol{V_P}'$ in equation (3. 1. 1).

The sets of $\boldsymbol{t}_i$ of the non-primitive lattices are the subsets of the sets of $\boldsymbol{t}_i$ of the primitive lattices. Since all the lattice points should be translatively equivalent to one another, the centering vectors should also be translatively equivalent to one another. The translative equivalence is guaranteed if the cosets $(\boldsymbol{t}_i + \boldsymbol{V_P})$ in $\boldsymbol{V_P}''$ form a factor group, $[\boldsymbol{V_P}''/\boldsymbol{V_P}]$. The unit element of the factor group is $\boldsymbol{V_P}$ and the coset representative of the element is null vector.

It must be noticed that the non-primitive lattices are essentially of one-to-one correspondence to the primitive lattices, if the bases are chosen to span the unit cells. That non-primitive lattices are subgroups of the primitive lattice is due to special choice of the bases, we can reversely regard that the primitive lattice is the subgroup of the non-primitive lattices.

3. 2 Rotative-translative invariance of centering vectors

The conditions to be satisfied for the centering vectors t_i is the lattices should be invariant for the point group symmetry operations of the corresponding primitive lattices. Since the representations of a symmetry operation of a primitive lattice expressed by equation (2. 1. 1), (3. 1. 1) and (3. 1. 2) are of quite the same form, the centering vectors should satisfy the rotative-translative invariance. Then equation (2. 4. 3) becomes

$$\boldsymbol{R}^t \boldsymbol{t}_i \equiv \boldsymbol{t}_i (mod.\ 1/m). \tag{3. 2. 1}$$

Since bases of the lattice expressed by equation (3. 1. 2) are multiplied by m, the **1** in equation (2. 4. 3) should be divided by m.

When the subset of the lattice (3. 1. 2) is required to have translation symmetry of the original lattice, $(mod.\ \mathbf{1}/m)$ in equation (3. 2. 1) should be replaced by $(mod.\ \mathbf{1})$. The condition that the translation group expressed by (3. 1. 2) is invariant for the point group

symmetries becomes

$$\boldsymbol{R}^t\boldsymbol{t}_i \equiv \boldsymbol{t}_j \,(mod.\ 1). \qquad (3.\ 2.\ 3)$$

That is to say, the set of centering vectors, $\{\boldsymbol{t}_i\}$ is rotativetranslatively invariant for a point group.

When the number of the equivalent positions with a position is equal to the order of the point group of the crystal, the position is a general position. Since the position vectors of the equivalent positions with the general position do not form a group, the number of the equivalent positions must be less than the order of the point group. Then there must be one symmetry operation at least, except identity, satisfying

$$\boldsymbol{R}^t\boldsymbol{t}_i \equiv \boldsymbol{t}_i \,(mod.\ 1). \qquad (3.\ 2.\ 4)$$

The points satisfying equation (3. 2. 4) are called rotativetranslatively invariant points.

The rotative-translatively invariant points for the symmetry operations in Table 1 are listed in Table 2. The letters a, b and c in Table 2 indicate that the coordinates are indefinite.

Point-group symmetries can be divided into three categories with respect to rotative-translative invariance.

(1) The coordinates are limited within 0 or 1/2.

The symmetry operations are: A, D, E, F, M, N, R and T in symbols of Hurley (1951).

(2) The coordinates have fractions with denominator 3.

The symmetry operations are: B, $K = N^2 = Z^2$, $B^2 = S^2$ and M^2.

(3) The coordinates are fractions with denominator 5.

The symmetry operation is: L.

When a centering vector is rotative-translatively invariant for a subgroup of the holohedry, then there are rotationally equivalent vectors with the centering vector. The number of the cosets of the primitive lattice in the non-primitive lattice, excluding the coset with zero vector, is N/n, where N is the order of the holohedry and n is the order of the subgroup. The cosets are invariant for the trnaslation operations of the primitive lattice, hence, the cosets have translation symmetry of the primitive lattice.

The centering vectors of KU-centered lattice are generated by the following four rotatively equivalent but translatively not equivalent vectors, that is, not rotative-translatively equivalent vectors.

$\boldsymbol{t}_1 = [1/4\ \ 1/4\ \ 1/4\ \ 1/4]$, $\boldsymbol{t}_2 = [-1/4\ \ -1/4\ \ 1/4\ \ 1/4]$,
$\boldsymbol{t}_3 = [1/4\ \ -1/4\ \ -1/4\ \ 1/4]$ and $\boldsymbol{t}_4 = [-1/4\ \ 1/4\ \ 1/4\ \ -1/4]$.

The other centering vectors can be expressed by linear combinations of these four vectors. The number of the cosets becomes sixteen for this lattice. Thses many cosets are necessary for the set of the vectors to form a lattice. If this lattice is allowed, the lattices with the centering vector,

$[1/n\ 1/n\ 1/n\ 1/n]$

and its equivalent vectors can be lattices where n is any integer, since the representations of the symmetry operations are the same with the case of $n = 1/2$.

The KG-centered lattice is obtained by adding a centering vector,

$[1/4\ 1/4\ 0\ 1/2]$

to the G-centered lattice. When crystal system is 12, the rotatively equivalent vectors with the vector becomes 8, and there is a vector $[1/4\ 3/4\ 0\ 1/2]$. The addition of these two vectors becomes $[1/2\ 0\ 0\ 0]$, this vector halves the base $\boldsymbol{a}_1$. This kind of vectors can not be centering vectors.

All symmetry operations in the point group should bring the lattice points to the lattice points which are translatively equivalent to one another in a primitive lattice. For non-primitive lattices, there are not translatively equivalent lattice points with respect to the translation of the corresponding primitive lattices, for example, three kinds of lattice points of all-face centered lattices, which are translatively equvalent to the three centering lattice points are not translatively equivalent to one another with respect to the translation of the corresponding primitive lattices. There are symmetry operations which bring these not translatively equivalent lattice point to one another. The centering vectors are not rotative-translatively invariant for the symmetry operations.

3. 3. Similarity of centering vectors

To avoid confusions, the lattices expressed by the form of (3. 1. 2) are called centered lattices and the lattices formed by $\boldsymbol{V}_P$ are called the primitive lattices of the centered lattices, or shortly the primitive lattices.

Obtaining centered lattices is equivalent to obtaining the sets of centering vectors. Centering vectors from which all centering vectors belonging to the sets can be obtained by applying the point group symmetry operations to the vectors are called generating centering vectors of the sets. There are sets of the centering vectors which have more than one generating centering vector. All-face centered lattice of orthorhombic lattice is for this example. Then, a set of centering vectors can be divided into subsets which have respective generating vectors. Hence, we must find out the method which can derive this kind of centered lattices.

To find the method, three-dimensional lattices are to be studied. The sets of the centering vectors of cubic lattices are invariant for the three-fold rotations about the body-diagonals. Hence, the centering vectors of cubic lattices are equivalent to one another. The rotations exchange cyclically the three equivalent bases. The body-centered lattice of tetragonal lattice is invariant for the exchange of the two bases which form two-dimensional square lattice. This exchange is also a symmetry operation. The representations of symmetry operations are invariant by the transformations due to the symmetrical exchanges of the bases. There is another kind of the exchanges of the bases which transform invariantly the representations of

symmetry operations. The cyclical exchange of the bases of orthorhombic primitive lattice transform invariantly the representations of symmetry operations.

The present author calls that the bases are similar to each other, if the representations of symmetry operations are invariant by the exchanges of the bases. Transformations caused by the exchanges of the similar bases are called similar transformations, and the exchanges as similar operations. If the bases are equivalent to one another, the similar operations become the symmetry operations. Similar operations for a lattice form a group. Although similar operations are not symmetry operations, the sets of the vectors, the lattices, are invariant as a whole for similar operations. The sets of the lattice vectors of non-primitive lattices should be also invariant as a whole by the similar operations. This nature of a lattice is called the similarity of the lattice. The invariance of a set of centering vectors for the similar operations is called the similarity of the centering vectors.

A similar operation is one-to-one mapping of a lattice as a whole. When a similar operation is represented by $\boldsymbol{S}$, the exchanged basis $[\boldsymbol{b}]$ is given by $\boldsymbol{S}[\boldsymbol{a}]$ where $[\boldsymbol{a}]$ is the original basis, and the mapping is given by

$$\boldsymbol{n} \leftrightarrow \boldsymbol{S}^t \boldsymbol{n}, \tag{3. 3. 1}$$

where $\boldsymbol{n}$ is a lattice vector.

3. 4. Closure of centering vectors

Rotative-translative invariance of centering vectors reduces the possible number of centering vectors in a non-primitive lattice. Regrettably, we can not find out a basic principle that how many systems of centering vectors can exist in a non-primitive lattice. This principle is introduced as the form of a postulation in this article. Of course, this postulation is satisfied in two- and three-dimensional lattices.

The postulation for the centering vectors of a non-primitive lattice is that the centering vectors should be similar to one another, where symmetry operations are included in the similar operations. The similar centering vectors are linearly independent of one another, since the similar operations are exchanges of the independent bases. This postulation is called the closure of centering vectors in this article, since this postulation limits strictly the set of centering vectors. As seen in the case of KU-centered lattice, not similar centering vectors are possibly introduced for non-primitive lattices to form groups, if this postulation is not set.

The similar centering vectors are at quite similar situation to the primitive lattice with one another, and the numbers of the equivalent vectors obtained from the holohedry are the same. The closure of centering vectors closes centering vectors of a non-primitive lattice within those at similar situations to the primitive lattice.

The D-centered lattice has three centering vectors,

$$\boldsymbol{t}_1 = [1/2\ 0\ 0\ 1/2],\ \boldsymbol{t}_2 = [0\ 1/2\ 1/2\ 0] \text{ and } \boldsymbol{t}_3 = \boldsymbol{t}_1 + \boldsymbol{t}_2 .$$

The vector $\boldsymbol{t}_3$ is necessary together for $\boldsymbol{t}_1$ and $\boldsymbol{t}_2$ to form a group. The generating symmetry

operation of the holohedry of the lattice is E. The representation of E is invariant for the exchange of the first and second bases and the third and fourth bases. This exchange is a similar operation. The similar operation transforms $\boldsymbol{t}_1$ to $\boldsymbol{t}_2$, $\boldsymbol{t}_2$ to t_1 and $\boldsymbol{t}_3$ to itself. The three subgroups generated with the cosets $(\boldsymbol{t}_i+\boldsymbol{V}_P')$ $(i = 1$ to $3)$ have the same order. The subgroup generated $(\boldsymbol{t}_3+\boldsymbol{V}_P')$ is not similar to the other two subgroup. The closure excludes this centered lattice from the Bravais lattices.

Monoclinic all-face centered lattice in three-dimensional space can be excluded by this closure, although the transformed representations of symmetry operations are unimodular.

3. 5. Definition of Bravais lattices

The definition of the lattices is:

When the representations of symmetry operations belonging to the holohedry of a lattice with reduced bases are the most simple in comparing with those of the other lattices with the same holohedry, the lattice is called the primitive lattice.

The most simple representation of a symmetry operation is of the least sum of the square of the elements of the representation matrix. If two representations have the same sum, the representation with more diagonal elements is simpler. Representations of symmetry operations become unimodular matrices with the elements 0 or ± 1, if the basis is reduced. There are many reduced lattices with the same holohedry, but the lattices with the most simple representations are limited within very few, and these can be transformed one another by the exchanges of the bases.

The definition of non-primitive lattices is:

The lattices derived from a primitive lattices by addition of the lattice points which are translatively equivalent to the centering vectors which are rotative-translatively invariant for the symmetry operations of primitive lattice and eqivalent or similar to one another are called the non-primitive lattices derived from the primitive lattice.

The representations of symmetry operations of the rhombohedral system in three dimensional space are the most simple, when rhombohedral bases are adapted. The rhombohedral lattice is derived from the addition of rotative-translatively invariant point for three-fold rotations to the hexagonal lattice. The representations of the three-fold rotations bases on the hexagonal bases are not simpler than those based on the rhombohedral bases.

4. Types of non-primitive lattices

4. 1. Non-primitive lattices compatible with symmetry operations of category (1)

The non-primitive lattices with the generating symmetry operations of this category described by *B. B. N. W. Z.* are *S* (seitenflächen-zentriert), *I* (innenzentriert), *Z* (zentral-zentriert), *D* (doppert-seitenflächen-zentriert), *F* (flächen-zentriert), *G* (gemischt-zentriert *S, I*), *KG* (kombiniert-gemischt-zentriert), *U* (überall-seitenflächen-zentriert) and *KU*

(kombiniert-überall-seitenflächen-zentriert).

There are four, eight and sixteen translatively equivalent positions for the positions,

[1/2 1/2 0 0], [1/2 1/2 1/2 0] and [1/2 1/2 1/2 1/2],

respectively. If these four, eight and sixteen positions are rotatively equivalent for the holohedries of the lattices, then there are face-centered (S -centered of *B. B. N. W. Z.*), three-dimensional body centered (I -centered) and four-dimensional body-centered (Z -centered) lattices for the lattices, respectively. In addition, when the bases of primitive lattices are similar for the cyclic exchange of three bases, there are three-dimensional all-face-centered lattices (F -centered).

The other lattices of this type, *D*-, *G*-, *U*-, *KU*-, and *KG*- centered lattices, should be discarded.

4. 2. Non-primitive lattices compatible with symmetry operations of Category (2)

This types of non-primitive lattices of *B. B. N. W. Z.*. are R (rhomboedrisch-zentriert), RR_1 (rhomboedrisch-rhomboedrisch-zentriert), RR_2 (rhomboedrisch-rhomboedrisch-zentriert) and RS (rhomboedrisch-seitenflächen-zentriert).

Rotative-translatively invariant points exist for only operations related with three-fold rotation operations. The possible centering vectors related with three-fold rotations are:

(i) [2/3 1/3 0 0].
(ii) [2/3 1/3 1/3 0].
(iii) [2/3 1/3 2/3 1/3].
(iv) [2/3 1/3 1/3 2/3].

When the bases are hexagonal-like, the number 2/3 in (i), (ii) and (iii) is replaced by [1/3] and the vector (iv) becomes [1/3 1/3 2/3 2/3] .

The vector (i) does not change the representations of symmetry operations, hence there is no non-primitive lattices with the centering vectors of this kind. The non-primitive lattice with the centering vector of the kind (ii) is R -centered lattice of *B. B. N. W. Z.* and analogous to the rhombohedral lattice of three-dimensional space. This non-primitive lattice occurs in the case of generating operation being K . The vectors (iii) and (iv) are invariant for the symmetry operations S^2 . The vector (iv) is not translatively equivalent to the vector (iii). The non-primitive lattice with the centering vector (iv) is different from that with the vector (iii).

We can not understand the centering vectors of the RR_1 - and RR_2 -centered lattices described by *B. B. N. W. Z.*, since the bases of the primitive lattice of the crystal system 17 of *B. B. N. W. Z.* (abbreviated as *C. S.* 17 hereafter, similarly abbreviated for the other crystal systems) are trigonal-like but the centering vector of RR_1 -centered lattice is given by [1/3 1/3 1/3 1/3] and the bases of the primitive lattice of *C. S.* 29 are hexagonal-like but the centering vector is [1/3 2/3 2/3 1/3] .

The present author denotes that the non-primitive lattices with the centering vector (iii) as RR_1-centered lattices and those with the vector (iv) as RR_2-centered lattices. This denotation may be different from that of *B. B. N. W. Z.*, it would not arise confusion if the difference is noticed.

The most easy and sure way to determine the non-primitive lattices of these kinds is to calculate the rotatively equivalent vectors with a assumed centering vector. If the rotatively equivalent vectors are all translatively equivalent, then the vector is to be the centering vector.

4. 3. Non-primitive lattice compatible with symmetry operations of Category (3)

Only one symmetry operation L belongs to this category. The invariant points are

$[n/5\ 2n/5\ 3n/5\ 4n/5]$ $(n = 1$ to $4)$.

The symmetry operation is transformed invariantly by the change of the basis to the above four vectors and their rotatively equivalent ones. The centering vector [1/5 2/5 3/5 4/5] does not satisfy rotative-translative invariance for the other member of *C.S.* 31, hence, there is no non-primitive lattice for the centering vectors.

5. Bravais lattices

5. 1. Primitive lattices

To derive primitive lattices, the holohedries must be determined correctly. It seems to be reexamined for the holohedries of *B. B. N. W. Z.*, since some holohedries contradict with the nature of lattices.

If the representation matrix of a symmetry operation is a direct sum of principal minor matrices, the subspaces corresponding to the minor matrices should be perpendicular to one another, because the subspaces transform to themselves by the operation and a subspace can be transformed by inversion without changing the other subspaces. For example, the generating operation of the holohedry of *C.S.* 10 is the operation D. The representation of D is the direct sum of two two-dimensional four-fold rotations. The primitive lattice is composed of two two-dimensional sublattices. If one of the sublattices is spanned by $\boldsymbol{a}$ and $\boldsymbol{b}$, then $-\boldsymbol{a}$ and $-\boldsymbol{b}$ can span the sublattice. The operation E must be an element of the group. Hence, the *C.S.* 10 is not a holohedry of the lattice.

In order to determine primitive lattices, the symmetry operations of the holohedries of crystal systems should be properly obtained. In addition, the lists of the symmetry operations of *B. B. N. W. Z.* are not directly available by themselves. The present author deduced the symmetry operations from the lists, the results are listed in Table 3. The matrices expressed in the Table 3 are given in Table 4. The *C.S.* 33 could not be examined by the personal computer in the present author's laboratory. The sets of representations of symmetry operations of crystal systems agree with the sets of those given by *B. B. N. W. Z.* as a whole, except *C.S.s*

27, 28 and 31. The *C.S.* 27 of *B. B. N. W. Z.* agrees with the set obtained by the present author's representations, when the matrices are transposed. The *C.S.* 28 agrees with the set of the present authors by transposing and exchanging the second and third axes. The *C.S.* 31 agrees with the set of the present authors by transposing and exchanging cyclically the first, second and third axes. The set of the present author's representations agrees with the set of crystal class 31/07/02 . This means that the crystal classes 31/07/01 and 31/07/02 of *B. B. N. W. Z.* are the same group.

The *C.S.* 5 is clearly a subgroup of the *C.S.* 6. The *C.S.* 8 is a subgroup of the *C.S.* 9. The transformation of bases to *R* -centered lattice proposed by *B. B. N. W. Z.* do not change the representations of symmetry operations to the unimodular ones. The *C.S.s* 10, 16 and 18 are the subgroups of the *C.S.* 19, since their lattices consist of two two-dimensional square lattices. The same relation exists in the *C.S.s* 11, 21, 22 and 23. The *C.S.* 12 is a subgroup of the *C.S.* 13. The *C.S.* 17 is a subgroup of the *C.S.* 23. One of the generating operations of the *C.S.* 17 is double two-dimensional three-fold rotation. The *C.S.* 17 becomes a holohedry owing to the rhombohedral lattice. The *C.S.* 24 is a subgroup of the *C.S.* 25. The *C.S.* 27 is a subgroup of the *C.S.* 31. But, the generating operation *L* is purely four-dimensional and the lattice having the symmetry of the *C.S.* 27 differs from that having the symmetry of the *C.S.* 31. The *C.S.s* 28 and 29 are subgroups of the *C.S.* 30. The *C.S.* 29 becomes the holohedry owing to the existence of the non-primitive lattice. The total number of the primitive lattices becomes 18. The metric tensors of the primitive lattices are given in Table 5. They are the same as those of *B. B. N. W. Z.* for the corresponding *C.S.s*

Primitive lattices are obtained by reducing the metric tensors to satisfy $\boldsymbol{RM} = \boldsymbol{M}(\boldsymbol{R}^t)^{-1}$. This reduction can be carried out easily and surely by the use of word processors.

5. 2. Non-primitive lattices

The non-primitive lattices to be examined are *S*, *I*, *Z*, *F*, *R*, RR_1 and RR_2.

C.S. 1. There is no non-primitive lattice.

C.S. 2. There is *S* -centered lattice.

C.S. 3. There is *S* -centered lattice.

C.S. 4. There are *S* -, *I* -centered lattices. *F* -centered lattice violates similarity.

C.S. 5. This crystal system should be merged to *C.S.* 6.

C.S. 6. There are *S* -, *I* -, *Z* -, *F* -centered lattices.

C.S. 7. There is *I* -centered lattice.

C.S. 8. There is no non-primitive lattice. This crystal system should be merged to *C.S.* 9. As seen from Table 3, this crystal system has a generating symmetry operation T_e'. This operation change the third and fourth coordinates, so that the two vectors

[0 1/3 2/3 1/3] and [0 1/3 1/3 2/3]

are rotatively equivalent. These two vectors are translatively not equivalent. If the former vector is a centering vector, then the latter vector should be also the centering vector. Then,

the vector [0 2/3 0 0] must be the centering vector, this contradict the translation symmetry of primitive lattice. The representations of symmetry operations can not be transformed to unimodular matrices.

C.S. 9. There is no non-primitive lattice.

C.S. 10. This crystal system should be merged to *C.S.* 19.

C.S. 11. This crystal system should be merged to *C.S.* 23.

C.S. 12. This crystal system should be merged to *C.S.* 13.

C.S. 13. There are S-, I-, Z-centered lattices.

C.S. 14. The primitive lattice agrees with that of *C.S.* 15.

There is R-centered lattice.

C.S. 16. This crystal system should be merged to *C.S.* 19.

C.S. 17. There are two pairs of rotatively equivalent points for the rotative-translatively invariant points,

(1) [2/3 1/3 2/3 1/3], [1/3 2/3 1/3 2/3],
(2) [2/3 1/3 1/3 2/3], [1/3 2/3 2/3 1/3].

These pairs of the vectors can be the centering vectors so that there are RR_1- and RR_2-centered lattices.

C.S. 18. This crystal system should be merged to *C.S.* 19.

C.S. 19. There is Z-centered lattice.

C.S. 20. There is no non-primitive lattice.

C.S. 21. This crystal system should be merged to *C.S.* 23.

C.S. 22. This crystal system should be merged to *C.S.* 23.

RR_2-centered lattice is proposed by *B. B. N. W. Z.* The rotatively equivalent vectors with the vector [1/3 1/3 2/3 2/3] are:

[1/3 1/3 1/3 1/3], [2/3 2/3 2/3 2/3]
[1/3 1/3 2/3 2/3], [2/3 2/3 1/3 1/3].

If the vector [1/3 1/3 2/3 2/3] is taken as the centering vector, then the vector [1/3 1/3 1/3 1/3] must be one of the centering vectors. Then these centering vectors violate the similarity, since the vector [2/3 2/3 0 0] should be the centering vector.

C.S. 23. There is no non-primitive lattice.

C.S. 24. This crystal system should be merged to *C.S.* 25.

C.S. 25. There are I-, Z- and F-centered lattices.

C.S. 26. There is no non-primitive lattice.

C.S. 27. There is no non-primitive lattice.

C.S. 28. This crystal system should be merged to *C.S.* 30.

C.S. 29. There is a non-primitive lattice. The centering vector is [1/3 1/3 1/3 1/3], that is, the vector (iii) in 4. 2. The centered lattice becomes RR_1-centered lattice by the notation of the present article..

C.S. 30. There is no non-primitive lattice.

C.S. 31. The centering vectors of *SN*-centered lattice are given by *B. B. N. W. Z.* are

[1/5 1/5 1/5 2/5], [1/5 1/5 2/5 1/5],
[1/5 2/5 1/5 1/5] and [2/5 1/5 1/5 1/5].

Thses four vectors are equivalent to one another, but the total number of equivalent vectors of these vectors is forty. The lattice spanned by the four vectors is different from the lattice with the forty centering vectors. This can be shown easily by comparing the points generated by the linear combination of the four vectors.

C.S. 32. The non-primitive lattice of this system is body-centered lattice and the lattice is said to have more symmetry than the system. The body-centered lattice is that of *C.S.* 33. The lattice was not examined. This lattice is counted as the approved.

5. 3. Summary of Bravais lattices

The primitive and non-primitive lattices derived by the present author's method are listed in Table 6. The crystal systems are due to *B. B. N. W. Z.* The double circles in Table 6 indicate that the lattices of *B. B. N. W. Z.* are approved by the present author. The single circles indicate that the lattices are proposed by the present author. The crosses indicate that the lattices of *B. B. N. W. Z.* are discarded by the method of the present author.

The number of crystal systems proposed in this paper becomes 20. Eighteen crystal systems correspond to the 18 primitive lattices, two crystal systems are obtained from the no-primitive lattices.

6. Discussions

The present author introduced the three principles to obtain centering vectors of non-primitiye lattices:

(1) Rotative-translative invariance of the centering vectors for the primitive lattices.

(2) Similarity of the centering vectors.

(3) Closure of the centering vectors.

The method to obtain centered lattices from a primitive lattice is as follows. At first, possible centering vectors for the holohedry are obtained by the rotative-translative invariance. The centering vectors are classified into sets of centering vectors according to the similarity. Then, the sets of similar centering vectors are tested to be the set of coset representatives, and the sets which are not closed in themselves to be coset representatives are excluded by the closure.

The geometrical method of derivation of non-primitive lattices described by Burckhardt (1966) presupposes evidently the principle (1).

Mackay and Pawley (1963) described the restrictions for the centering vectors as follows.

(1) The point-group symmetry at each lattice point must be the same as in the uncentred lattice.
(2) Every lattice point must have the same environment.
(3) Halving of translation merely gives the same lattice.
(4) The coordinates of the lattice points form a group closed with respect to addition and subtraction (mod. 1)

The restriction (1) is satisfied if the principle (1) is satisfied. Quantitative criterion for the restriction (2) is lack in their method. The present author introduced the closure of centering vectors for this purpose. The restrictions (3) and (4) are the direct results of the condition on the translation groups described in this article.

The only apparently reliable method to derive non-primitive lattices until now is as follows. The set of the representations of symmetry operations of the holohedry of a lattice with reduced bases is denoted by G. There are two kinds of transformation matrices in equation (2. 2. 4) which transform the representations to the unimodular matrices, the one kind is that the transformation matrices are unimodular, the matrices are denoted by $\boldsymbol{Us}$, the other kind is that the transformation matrices are singular matrices with the elements of fractional numbers, the matrices are denoted by $\boldsymbol{Ts}$. The former kind of transformations is of iso-volume, and the latter kind of transformations is not of iso-volume.

Two representations of a symmetry operation are said to be arithmetically equivalent, when the representations are transformed to each other by the former kind of transformation. Two representations are said to be geometrically equivalent when the transformation is of the latter kind.

The set, S, of all the unimodular representations of symmetry operations of the holohedry can be classified into the subsets of the unimodular representations of the symmetry operations, the subsets are geometrically equivalent to one another,

$$S = \{\boldsymbol{URU}^t : \boldsymbol{R} \in G\} U \{\boldsymbol{URU}^t : \boldsymbol{R} \in \boldsymbol{TGT}^t\} U \ldots\ldots$$

where $\boldsymbol{TGT}^t = \{\boldsymbol{TRT}^t : \boldsymbol{R} \in G\}$, that is, the set of the representations of the holohedry transformed by a matrix $\boldsymbol{T}$, and $\{\boldsymbol{URU}^t : \boldsymbol{R} \in \boldsymbol{TGT}^t\}$ means that the set of the representations arithmetically equivalent to the members of $\boldsymbol{TGT}^t$. Although there are infinite many equivalent transformations with a $\boldsymbol{T}$, these can be expressed by $\boldsymbol{UTU}^t$, and the representations transformed by $\boldsymbol{UTU}^t$ are contained in the set $\{\boldsymbol{URU}^t : \boldsymbol{R} \in \boldsymbol{TGT}^t\}$.

The number of the distinct subsets $\{\boldsymbol{URU}^t : \boldsymbol{R} \in \boldsymbol{TGT}^t\}$ which are not arithmetically equivalent to one another is assumed to be the number of non-primitive lattices.

According to this method, the D-centered lattice can be a Bravais lattice. But, this method fails to exclude the All-face centered lattices of monoclinic and tetragonal lattices, since the holohedry of the monoclinic lattice is a subgroup of that of the orthorhombic lattice, and the tetragonal one is a subgroup of that of the cubic one, the representations of the symmetry operations of both the All-face centered lattices become the unimodular matrices.

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Table 1. The symmetry operation in [4] After Mackay & Pawley (1963)

Multiplicity m	$(\chi, \sigma, \lvert T_{ij} \rvert)$	Hurley's letter	Hermann's symbol	Matrix
1	(4, 6, 1)	I	1111	$\begin{pmatrix} 1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1 \end{pmatrix}$
8	(0, 0, 1)	A	8	$\begin{pmatrix} 0&1&0&0\\0&0&1&0\\0&0&0&1\\-1&0&0&0 \end{pmatrix}$
6	(0, 1, 1)	B	63	$\begin{pmatrix} 0&-1&0&0\\1&1&0&0\\0&0&0&1\\0&0&-1&-1 \end{pmatrix}$
12	(0, −1, 1)	C	T	$\begin{pmatrix} 0&0&0&1\\0&0&-1&-1\\0&-1&0&0\\1&1&0&0 \end{pmatrix}$
4	(0, 2, 1)	D	44	$\begin{pmatrix} 0&1&0&0\\-1&0&0&0\\0&0&0&1\\0&0&-1&0 \end{pmatrix}$
2	(0, −2, 1)	E	2211	$\begin{pmatrix} -1&0&0&0\\0&-1&0&0\\0&0&1&0\\0&0&0&1 \end{pmatrix}$
4	(0, 0, −1)	F	421	$\begin{pmatrix} 0&1&0&0\\-1&0&0&0\\0&0&-1&0\\0&0&0&1 \end{pmatrix}$
3	(1, 0, 1)	K	311	$\begin{pmatrix} 0&1&0&0\\-1&-1&0&0\\0&0&1&0\\0&0&0&1 \end{pmatrix}$
5	(1, 1, 1)	L	5	$\begin{pmatrix} 0&1&0&0\\0&0&1&0\\0&0&0&1\\-1&-1&-1&-1 \end{pmatrix}$
12	(1, 2, 1)	M	64	$\begin{pmatrix} 0&-1&0&0\\1&1&0&0\\0&0&0&-1\\0&0&1&0 \end{pmatrix}$
6	(1, 0, −1)	N	621	$\begin{pmatrix} 0&-1&0&0\\1&1&0&0\\0&0&-1&0\\0&0&0&1 \end{pmatrix}$
4	(2, 2, 1)	R	411	$\begin{pmatrix} 0&1&0&0\\-1&0&0&0\\0&0&1&0\\0&0&0&1 \end{pmatrix}$
6	(2, 3, 1)	S	66	$\begin{pmatrix} 0&-1&0&0\\1&1&0&0\\0&0&0&-1\\0&0&1&1 \end{pmatrix}$
2	(2, 0, −1)	T	2111	$\begin{pmatrix} -1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1 \end{pmatrix}$
6	(3, 4, 1)	Z	611	$\begin{pmatrix} 0&-1&0&0\\1&1&0&0\\0&0&1&0\\0&0&0&1 \end{pmatrix}$

Table 2. Rotative-translatively invariant points

Symmetry operation	Rotative-translatively invariant point			
A	1/2	1/2	1/2	1/2
B	0	0	2/3	1/3
	0	0	1/3	2/3
C	0	0	0	0
D	0	0	1/2	1/2
	1/2	1/2	0	0
	1/2	1/2	1/2	1/2
E	1/2	0	a	b
	0	1/2	a	b
	1/2	1/2	a	b
F	0	0	1/2	a
	1/2	1/2	1/2	a
K	2/3	1/3	a	b
	1/3	2/3	a	b
L	1/5	2/5	3/5	4/5
	2/5	4/5	1/5	3/5
	3/5	1/5	4/5	2/5
	4/5	3/5	2/5	1/5
M	0	0	1/2	1/2
N	0	0	1/2	a
R	1/2	1/2	a	b
S	0	0	0	0
T	1/2	a	b	c
Z	0	0	0	0
S^z	2/3	1/3	0	0
	1/3	2/3	0	0
	0	0	2/3	1/3
	0	0	1/3	2/3
	1/3	2/3	1/3	2/3
	1/3	2/3	2/3	1/3
	2/3	1/3	2/3	1/3
	2/3	1/3	1/3	2/3

Table 3. Crystal systems and generating operations

Crystal sestem	Order of group	Generating operations of holohedry
1	2	-I
2	4	-I, T"'
3	4	-I, E
4	8	-I, T"', T"
5	8	-I, E, E'
6	16	-I, E, E', T
7	16	-I, R', T"'
8	12	-I, K', T_e'
9	24	-I, Z', T_e'
10	4	D
11	6	S
12	16	-I, F', E"
13	32	-I, F', E", T"
14	24	-I, K', T, T"'$_e$
15	48	N', -E, T, T_e'
16	8	D, E"
17	12	-I, S_t^2, E"$_e$
18	32	D, E, T", T_e
19	64	D, E, E", T_e, T"'
20	96	-I, N', R, E'$_e$
21	24	S_h, E, E"$_h$
22	72	S_h, K_h, T_e', T"'$_e$'
23	144	S_h, K_h, E, T_e, T"'$_e$
24	48	-I, K_d', E', E", T'$_e$
25	96	-I, K_d', E', E", T'$_e$, T
26	16	A, E_d
27	20	-I, L, E_d
28	24	S_h, K_h, E"'$_e$, E_d
29	144	-I, S_h^2, K_h, E"$_e$, E_d, T_e
30	288	S_h, K_h, E"$_e$, E_d, T_e, E
31	240	-I, L, F", K_d, T'$_e$
32	384	D, F, K_d, E_d, E"$_e$, T
33	1152	?

Table 4. Representations of symmetry operations used in Table 3.

T'
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

T"
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

T"'
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

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

T'$_e$
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

T_e'
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

T"'$_e$'
$$\begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

T"'$_e$
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

E'
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

E"
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

E"$_e$
$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

E"'$_e$
$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

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

E"$_h$
$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix}$$

F'
$$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}$$

$$F'' \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad K' \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & -1 \end{pmatrix} \quad K_h \begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$K_d \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad K_d' \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad S_h \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 1 \end{pmatrix}$$

$$S_t \begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \quad B' \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{pmatrix} \quad N' \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

$$R' \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \quad Z' \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

Table 5. Metric tensors of primitive lattices four dimensional space

Crystal system	Metric tensor	Crystal system	Metric tensor
1	$\begin{pmatrix} a_1^2 & a_1a_2 & a_1a_3 & a_1a_4 \\ & a_2^2 & a_2a_3 & a_2a_4 \\ & & a_3^2 & a_3a_4 \\ & & & a_4^2 \end{pmatrix}$	2	$\begin{pmatrix} a_1^2 & a_1a_2 & a_1a_3 & 0 \\ & a_2^2 & a_2a_3 & 0 \\ & & a_3^2 & 0 \\ & & & a_4^2 \end{pmatrix}$
3	$\begin{pmatrix} a_1^2 & a_1a_2 & 0 & 0 \\ & a_2^2 & 0 & 0 \\ & & a_3^2 & a_3a_4 \\ & & & a_4^2 \end{pmatrix}$	4	$\begin{pmatrix} a_1^2 & a_1a_2 & 0 & 0 \\ & a_2^2 & 0 & 0 \\ & & a_3^2 & 0 \\ & & & a_4^2 \end{pmatrix}$
5, 6	$\begin{pmatrix} a_1^2 & 0 & 0 & 0 \\ & a_2^2 & 0 & 0 \\ & & a_3^2 & 0 \\ & & & a_4^2 \end{pmatrix}$	7	$\begin{pmatrix} a_1^2 & a_1a_2 & 0 & 0 \\ & a_2^2 & 0 & 0 \\ & & a_3^2 & 0 \\ & & & a_3^2 \end{pmatrix}$
9	$\begin{pmatrix} a_1^2 & a_1a_2 & 0 & 0 \\ & a_2^2 & 0 & 0 \\ & & a_3^2 & a_3^2/2 \\ & & & a_3^2 \end{pmatrix}$	12, 13	$\begin{pmatrix} a_1^2 & 0 & 0 & 0 \\ & a_2^2 & 0 & 0 \\ & & a_3^2 & 0 \\ & & & a_3^2 \end{pmatrix}$
15	$\begin{pmatrix} a_1^2 & 0 & 0 & 0 \\ & a_2^2 & 0 & 0 \\ & & a_3^2 & a_3^2/2 \\ & & & a_3^2 \end{pmatrix}$	10, 16, 18, 19	$\begin{pmatrix} a_1^2 & 0 & 0 & 0 \\ & a_1^2 & 0 & 0 \\ & & a_2^2 & 0 \\ & & & a_2^2 \end{pmatrix}$
20	$\begin{pmatrix} a_1^2 & 0 & 0 & 0 \\ & a_1^2 & 0 & 0 \\ & & a_2^2 & a_2^2/2 \\ & & & a_2^2 \end{pmatrix}$	11,17,21,22,23	$\begin{pmatrix} a_1^2 & -a_1^2/2 & 0 & 0 \\ & a_1^2 & 0 & 0 \\ & & a_2^2 & -a_2^2/2 \\ & & & a_2 \end{pmatrix}$
24, 25	$\begin{pmatrix} a_1^2 & 0 & 0 & 0 \\ & a_2^2 & 0 & 0 \\ & & a_2^2 & 0 \\ & & & a_2^2 \end{pmatrix}$	26	$\begin{pmatrix} a_1^2 & a_1a_2 & 0 & -a_1a_2 \\ & a_1^2 & a_1a_2 & 0 \\ & & a_1^2 & a_1a_2 \\ & & & a_1^2 \end{pmatrix}$
27	$\begin{pmatrix} a_1^2 & a_1a_2 & -a_1^2/2-a_1a_2 & -a_1^2/2-a_1a_2 \\ & a_1^2 & a_1a_2 & -a_1^2/2-a_1a_2 \\ & & a_1^2 & a_1a_2 \\ & & & a_1^2 \end{pmatrix}$	28, 29, 30	$\begin{pmatrix} a_1^2 & -a_1^2/2 & 0 & 0 \\ & a_1^2 & 0 & 0 \\ & & a_1^2 & -a_1^2/2 \\ & & & a_1^2 \end{pmatrix}$
31	$\begin{pmatrix} a_1^2 & -a_1^2/4 & -a_1^2/4 & -a_1^2/4 \\ & a_1^2 & -a_1^2/4 & -a_1^2/4 \\ & & a_1^2 & -a_1^2/4 \\ & & & a_1^2 \end{pmatrix}$	32	$\begin{pmatrix} a_1^2 & 0 & 0 & 0 \\ & a_1^2 & 0 & 0 \\ & & a_1^2 & 0 \\ & & & a_1^2 \end{pmatrix}$

Table 6. Crystal systems and Bravais Lattices

C.S.	P	S	I	Z	F	R	D	U	G	RR_1	RR_2	SN	KU	KG	RS
01	◎														
02	◎	◎													
03	◎	◎					+								
04	◎	◎	◎		+		+								
05													+		
06	◎	◎	◎	◎	◎		+	+	+						
07	◎		◎												
08						+									
09	◎														
12														+	
13	◎	◎	◎	◎					+						
14						◎									+
15	◎	◎													
17										◎	○				
19	◎			◎			+								
20	◎														
22											+				
23	◎														
24													+		
25	◎		◎	◎	◎			+							
26	◎														
27	◎														
29										○	+				
30	◎														
31	◎											+			
32	◎														
33				(◎)											

Table 7. Crystal systems and primitive lattices

Crystal system	Order of group	B.B.N.W.Z.	Mackay & Pawley	Kuntsevich & Below	Takahashi
1	2	○	1	1	○
2	4	○	2	2	○
3	4	○	3	3	○
4	8	○	4	4	○
5	8				
6	16	○	7	5	○
7	16	○	6	6	○
8	12				
9	24	○	5	9	○
10	4	○		17	
11	6	○		18	
12	16			8	
13	32	○	10	7	○
14	24				
15	48	○	11	11	○
16	8	○	8	19	
17	12	○		20	
18	32				
19	64	○	14	21	○
20	96	○	13	15	○
21	24				
22	72				
23	144	○	15	16	○
24	48				
25	96	○	12	13	○
26	16	○	?	?	○
27	20	○	?	?	○
28	24	○	17	24	
29	144				
30	288	○	19	25	○
31	240	○	21	26	○
32	384	○	20	22	○
33	1152				