Reduced cells of Bravais Lattices

Hidewo TAKAHASHI

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Abstract

Reduction conditions of ternary quadratic forms given by Eisenstein [*J. Math.*(1851), 41, 141-190] and adopted in *International Tables for Crystallography*, Vol. A are discussed to be unsuitable for the reduction conditions of Bravais lattices. Electronic computer program for obtaining the reduced cells from any given Bravais lattices is made and the forty four reduced cells in the *Tables* are examined. The three kinds of errors or defects due to the reduction conditions or their application are found by the examination. They are:

(1) Trivial error, No. 18 cell in the *Tables*;

(2) Violation of the principle of classification, No. 1, 9 and 24 cells in the *Tables*;

(3) Violation of the translation symmetry, No. 43 cell in *Tables*.

1. Introduction

Reduced cells were introduced by Niggli (1982), and listed in *International Tables for Crystallography* (1983), Vol. A, (abridged by I. T. hereafter). His method depended on the results of the reduction of ternary quadratic forms of Eisenstein (1851). If we can know all the ternary quadratic forms corresponding to Bravais lattices a *priori*, or if any ternary quadratic form necessarily corresponds to a Bravais lattice, we might obtain Bravais lattices from the reduced cells. Many crystallographers imagined that the best way to obtain Bravais lattices were to obtain the reduced cells at first. Even Burckhardt (1966) described as if symmetry operations could be obtainable from the reduced cells in two dimensional space. But, he could not extrapolate naturally the method to three dimensional space. The reduction of ternary quadratic forms is to obtain the shortest and the nearest bases to the orthogonal bases by exchange of the bases by linear combinations with integral coefficients of the bases, and does not give any other new information than that included in the starting bases.

The condition (2. a) in I. T. has the ambiguity that the both cells of type-I and type-II satisfy the same condition. Since lattice points $\boldsymbol{b}$ and $(\boldsymbol{b}+\boldsymbol{a})$ are translationally equivalent with each other when $\boldsymbol{a}\cdot\boldsymbol{b} = a^2/2$ in case of $a^2 < b^2$, we can not determine the types of cells with $\boldsymbol{a}\cdot\boldsymbol{b} = -a^2/2$. Face-centered cubic cell can be spanned by $(\boldsymbol{a}+\boldsymbol{b})/2$, $(-\boldsymbol{a}+\boldsymbol{b})/2$ and $(-\boldsymbol{b}+\boldsymbol{c})/2$, then the cell is reduced and becomes type-II, although the cell is classified to be

Faculty of Education Kagoshima University

type-I in I. T.

Křivý and Gruber (1976) proposed an algorithm for determining the reduced cells. The program written by Quick BASIC was made by the present author along their algorithm. Face-centered cubic cell became type-I by their algorithm, and could not be reduced further.

The present authour made new program written by Quick BASIC by taking into consideration of their algorithm and their result was tested by the program. The elements of the metric tensor of their reduced cell given for an example were $A=4$, $B=C=9$, $\xi=9$, $\eta=3$ and $\zeta=4$. The elements obtained by the present author's method are $A=4$, $B=9$, $C=9$, $\xi=-8$, $\eta=-1$, and $\zeta=-4$. The basis vectors are $\boldsymbol{a}'=\boldsymbol{a}$, $\boldsymbol{b}'=\boldsymbol{b}-\boldsymbol{a}$, $\boldsymbol{c}'=\boldsymbol{c}-\boldsymbol{b}$, where $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ are their basis vectors.

All the reduced cells were examined from theoretical and numerical points of view. In the course of the examination, some wrong reduced cells were found in I. T.

2. Ternary quadratic forms

Ternary quadratic form means that the set of numbers which are expressed by the following form,

$$\phi(n_1, n_2, n_3) = n_1^2 a_{11} + n_2^2 a_{22} + n_3^2 a_3^2 + 2(n_1 n_2 a_{12} + n_2 n_3 a_{23} + n_3 n_1 a_{31}). \tag{2.1}$$

The expression (2.1) can be rewritten by using matrices $\boldsymbol{n}^t = [n_1\ n_2\ n_3]$ and $\boldsymbol{M} = [a_{ij}]$ by

$$\phi(n_1, n_2, n_3) = \boldsymbol{n}^t \boldsymbol{M} \boldsymbol{n}, \tag{2.2}$$

where the superscript "t" indicates "transposed matrix of" and a_{ij} is the ij element of the matrix $\boldsymbol{M}$. The matrix $\boldsymbol{M}$ is called metric tensor.

A set L of all crystal lattice vectors is expressed by

$$L = \{n_1 \boldsymbol{a} + n_2 \boldsymbol{b} + n_3 \boldsymbol{c}; -\infty < n_1, n_2, n_3 < \infty\}. \tag{2.3}$$

The basis vectors $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ can be chosen infinite many ways if the basis vectors span the lattice. Square of a lattice vector v becomes

$$v^2 = n_1^2 a^2 + n_2^2 b^2 + n_3^2 c^2 + 2(n_1 n_2 \boldsymbol{a}\cdot\boldsymbol{b} + n_2 n_3 \boldsymbol{b}\cdot\boldsymbol{c} + n_3 n_1 \boldsymbol{c}\cdot\boldsymbol{a}). \tag{2.4}$$

Comparing equation (2.1) with (2.4), the set of squared lattice vectors becomes a ternary quadratic form. The squared lattice vectors can be expressed by

$$v^2 = \boldsymbol{n}^t \boldsymbol{M} \boldsymbol{n} \tag{2.5}$$

where $\boldsymbol{n}^t = [\boldsymbol{n}_1\ \boldsymbol{n}_2\ \boldsymbol{n}_3]$ and $\boldsymbol{M}$ is given by

$$\boldsymbol{M} = [a][a]^t, \tag{2.6}$$

where the matrix $[a]^t$ is $[\boldsymbol{a}\ \boldsymbol{b}\ \boldsymbol{c}]$.

3. Conditions of reduced cell

To make the off-diagonal elements of the metric tensor M be possibly smaller by keeping the quadratic form unchanged, that is, the set of the numbers is unchanged by the change of the elements, is called reduction of quadratic forms.

According to I. T., reduced cells are classified into two type, type-I and type-II, by the sign of T,

$$T = (\boldsymbol{a}\cdot\boldsymbol{b})(\boldsymbol{b}\cdot\boldsymbol{c})(\boldsymbol{c}\cdot\boldsymbol{a}), \tag{3. 1}$$

where $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ are a (reduced or not) basis of the lattice. For the type-I cell, the main coditions are:

$$\boldsymbol{a}\cdot\boldsymbol{a} \leq \boldsymbol{b}\cdot\boldsymbol{b} \leq \boldsymbol{c}\cdot\boldsymbol{c}; |\boldsymbol{b}\cdot\boldsymbol{c}| \leq (\boldsymbol{b}\cdot\boldsymbol{b})/2; |\boldsymbol{a}\cdot\boldsymbol{c}| \leq (\boldsymbol{a}\cdot\boldsymbol{a})/2; |\boldsymbol{a}\cdot\boldsymbol{b}| \leq (\boldsymbol{a}\cdot\boldsymbol{a})/2 \tag{3. 2}$$

$$\boldsymbol{b}\cdot\boldsymbol{c} > 0;\ \boldsymbol{a}\cdot\boldsymbol{c} > 0;\ \boldsymbol{a}\cdot\boldsymbol{b} > 0. \tag{3. 3}$$

For the type-II cell, the main conditions are:
In addition to (3. 2),

$$(|\boldsymbol{b}\cdot\boldsymbol{c}| + |\boldsymbol{a}\cdot\boldsymbol{c}| + |\boldsymbol{a}\cdot\boldsymbol{b}|) \leq (\boldsymbol{a}\cdot\boldsymbol{a} + \boldsymbol{b}\cdot\boldsymbol{b})/2 \tag{3. 4}$$

$$\boldsymbol{b}\cdot\boldsymbol{c} \leq 0;\ \boldsymbol{a}\cdot\boldsymbol{c} \leq 0;\ \boldsymbol{a}\cdot\boldsymbol{b} \leq 0. \tag{3. 5}$$

These conditions were proposed by Eisenstein (1851).

Eisenstein's conditions, adapted in I. T., are ambiguous for the distinction of the types, since they do not decide uniquely the types of cells. Face-centered cubic lattice has reduced cells both type-I and type-II. The origin of the ambiguity is too elementary, because the equality in (3. 2) must be removed from the either condition of the two main conditions. If the value of $\boldsymbol{a}\cdot\boldsymbol{b}$ is equal to $\boldsymbol{a}\cdot\boldsymbol{a}/2$, the lattice point of which lattice vector $\boldsymbol{b}-\boldsymbol{a}$ is translationally equivalent to the lattice point of which lattice vector is $\boldsymbol{b}$. Hence, we must choose one of the vectors for basis vectors. Since axial angle ß of monoclinic lattice is obtuse and the angle γ of hexagonal lattice is $2\pi/3$, it is natural to put the equal symbol like in (3. 8). Then, the equal symbols in (3. 2) for the type-I should be removed.

According to Minkowski (1883), when we rewrite his notations in vector forms, the necessary and sufficient conditions are:

$$\boldsymbol{a}\cdot\boldsymbol{a} \leq \boldsymbol{b}\cdot\boldsymbol{b} \leq \boldsymbol{c}\cdot\boldsymbol{c} \tag{3. 6}$$

$$(\varepsilon_1\boldsymbol{a} + \varepsilon_2\boldsymbol{b} + \varepsilon_3\boldsymbol{c})^2 \geq A, \tag{3. 7}$$

where A is $\boldsymbol{a}\cdot\boldsymbol{a}$, $\boldsymbol{b}\cdot\boldsymbol{b}$ or $\boldsymbol{c}\cdot\boldsymbol{c}$ if ε_1, ε_2 or ε_3 is 1, respectively. We obtain necessary sufficient conditions from (3. 7):

$$-\boldsymbol{a}\cdot\boldsymbol{a}/2 \leq \boldsymbol{a}\cdot\boldsymbol{b} < \boldsymbol{a}\cdot\boldsymbol{a}/2; -\boldsymbol{b}\cdot\boldsymbol{b}/2 \leq \boldsymbol{b}\cdot\boldsymbol{c} < \boldsymbol{b}\cdot\boldsymbol{b}/2; -\boldsymbol{a}\cdot\boldsymbol{a}/2 \leq \boldsymbol{a}\cdot\boldsymbol{c} < \boldsymbol{a}\cdot\boldsymbol{a}/2 \tag{3. 8}$$

$$(\varepsilon_1\boldsymbol{a} + \varepsilon_2\boldsymbol{b} + \boldsymbol{c})^2 \geq \boldsymbol{c}\cdot\boldsymbol{c} \tag{3. 9}$$

where ε_1 and ε_2 are 0 or ± 1 . The condition (3. 9) shows that the condition (3. 4) for type-Ⅱ should be satisfied for both the type-Ⅰ and type-Ⅱ.

The bases and tensor elements are denoted as follows in the succeeding description. Basis vectors of the primitive cell of a Bravais lattice are denoted by $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$, where primitive cells mean the cells with the minimum volume of which apexes are at the lattice points. The basis vectors of a reduced cell are denoted by $\boldsymbol{a}'$, $\boldsymbol{b}'$ and $\boldsymbol{c}'$. The diagonal tensor elements are denoted by A, B and C , where $A = \boldsymbol{a}' \cdot \boldsymbol{a}'$, $B = \boldsymbol{b}' \cdot \boldsymbol{b}'$ and $C = \boldsymbol{c}' \cdot \boldsymbol{c}'$. The off-diagonal elements are denoted by D , E and F , where $D = \boldsymbol{b}' \cdot \boldsymbol{c}'$, $E = \boldsymbol{a}' \cdot \boldsymbol{c}'$ and $E = \boldsymbol{a}' \cdot \boldsymbol{b}'$.

4. Equivalence of reduced cell

There are two kinds of symmentries in metric tensors:

(1) Forms of the two metric tensors are the same;

(2) two metric tensors can be transformed to each other by suitable renumbering of the basis vectors.

The first kind of metric tensors are found in metric tensors of triclinic cells. The reduced cells of No. 31 and 44 in I. T. are of this kind. The second kind of metric tensors are those of monoclinic cells of No. 33, 34 and 35.

Two reduced cells satisfy (1) or (2) are symmetrically equivalent to one another. Symmetrically equivalent cells should be classified as the same cells.

5. Program of reduction

The main defects in the program written by the algorithm of Křivý and Gruber (1976) are:

(1) The reduced forms depend sometimes on the sequential order of the reduction of the two dimensional lattices (algorithm 5. 6. and 7.);

(2) The cells with equal lengths of basis vectors are not reduced sometimes.

The main part of their program lies in obtaining the vectors satisfying the two dimensional condition (3. 8). The former defect can be removed by adjusting three dimensionally the three vectors to satisfy the three dimensional condition (3. 9) after two dimensinoal reduction.

The latter defect can be removed by simplifying the algorithm 1. and 2. by eradicating the procedures for the diagonal tensor elements being equal. Their algorithm introduced groundless procedures in algorithm 1., 2. and 8.

The program were very simplified and the list of the program except subroutines which give the tensor elements of centered lattices is shown in Appendix.

6. Examination of the reduced cells of I. T.

Triclinic lattice

There is two reduced cells in I.T. These cells are equivalent to each other. They are numbered by 1.

Monoclinic lattices

(1) Primitive lattice

Since monoclinic axial angle ß is obtuse, when $c > a$, the angle should satisfy

$$0 > \cos \beta \geq -a/(2c),$$

where a and c are the absolute values of $\boldsymbol{a}$ and $\boldsymbol{c}$.

The basis vector $\boldsymbol{b}$ is unique, $\boldsymbol{a}$ and $\boldsymbol{c}$ can be set to be $c > a$. The possible combinations of order of the lengths of the basis vectors are (i) $b \geq c > a$, (ii) $c > b \geq a$ and (iii) $c > a \geq b$. These three bases are reduced, and are equivalent to one another. They are numbered by 2.

(2) C-centered lattice

The centered plane is assumed to be of C-face. The centering vectors $(\boldsymbol{a}+\boldsymbol{b})/2$ and $(-\boldsymbol{a}+\boldsymbol{b})/2$ are denoted by $\boldsymbol{t}_1$ and $\boldsymbol{t}_2$. The value of $\boldsymbol{c}$ can not be assumed to be larger than $\boldsymbol{a}$, so that there are two cases, $c \geq a$ and $a \geq c$. The primitive cells spanned by the basis vectors $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ are reduced, if the angle ß satisfies

$$\cos \beta \geq -a/(2c) \text{ for } c \geq a,$$

or

$$\cos \beta \geq -c/(2a) \text{ for } a \geq c,$$

Two dimensional lattice spanned by $\boldsymbol{c}$ and $\boldsymbol{t}_1$ are reduced, if

$$(\boldsymbol{c}+\boldsymbol{t}_1)^2 - c^2 > 0 \text{ for } c^2 > t_1^{\,2}\text{, that is, } \cos \beta > -(a^2+b^2)/(4ca),$$

or

$$(\boldsymbol{c}-\boldsymbol{t}_1)^2 - t_1^{\,2} > 0 \text{ for } t_1^{\,2} > c_2\text{, that is, } \cos \beta > -c/a.$$

Since $\cos \beta > -a/2c \; (c > a)$ or $-c/2a \; (a > c)$, the cell spanned by $\boldsymbol{c}$ and $\boldsymbol{t}_1$ can be reducible, if

$$-(a^2+b^2)/(4ca) > \cos \beta > -a/2c \text{ for } c > a,$$

or

$$-(a^2+b^2)/(4ca) > \cos \beta > -c/2a \text{ for } a > c.$$

There is no possibility for $(\boldsymbol{c}+\boldsymbol{t}_1)^2 < t_1^{\,2}$.

When $a^2 \geq t_1{}^2$, then $b^2/3 \geq a^2$, and when $b^2 \geq t_1{}^2$, then $3b^2 \geq a^2$. Hence, the range of a is divided into the four cases:

(i) $b^2/3 \geq a^2$;

(ii) $b^2 \geq a^2 > b^2/3$;

(iii) $3b^2 \geq a^2 > b^2$;

(iv) $a^2 > 3b^2$.

The cells spanned by $\boldsymbol{a}$, $\boldsymbol{t}_1$ and $\boldsymbol{c}$ are reduced in the case (i) and by $\boldsymbol{t}_1$, $\boldsymbol{t}_2$ and $\boldsymbol{c}$ in the case (ii). They are numbered by 3 and 4, respectively. The cell spanned by $\boldsymbol{t}_1$, $\boldsymbol{t}_2$ and $\boldsymbol{c}$ can be reducible if $a > c$ and $-(a^2+b^2)/(4ca) > \cos\beta > -c/(2a)$, and if $c > a$ and $-(a^2+b^2)/(4ca) > \cos\beta > -a/2c$ in (iii). Then, the basis vectors become $\boldsymbol{t}_1$, $\boldsymbol{t}_2$ and $\boldsymbol{c}+\boldsymbol{t}_1$, the reduced cell is numbered by 5. The other cells in this case are reduced, the cells are spanned by $\boldsymbol{t}_1$, $\boldsymbol{t}_2$ and $\boldsymbol{c}$, and are numbered by 4'. These cells are equivalent to cells of No. 4. The basis vectors become $\boldsymbol{b}$, $\boldsymbol{c}$ and $\boldsymbol{t}_1$ in (iv). The cells spanned by the basis vectors are reduced under the same condition in (iii). The cells spanned by $\boldsymbol{b}$, $\boldsymbol{c}$ and $\boldsymbol{t}_1$ are numbered by 6 and the cell spanned by $\boldsymbol{b}$, $\boldsymbol{t}_1$ and $\boldsymbol{c}+\boldsymbol{t}_1$ is numbered by 7.

The cell 43 in I. T. is not translationally equivalent to the cells of C-face centered lattices.

Orthorhombic lattices

(1) Primitive lattice

There is only one reduced cell and the cell is numbered by 8.

(2) C-face centered lattice

This lattice can be treated by simplifying the case of C-face centered monoclinic lattice. The basis vector $\boldsymbol{c}$ is always one of the basis vectors of the reduced cells. The other vectors are chosen from $\boldsymbol{a}$, $\boldsymbol{t}_1 = (\boldsymbol{a}+\boldsymbol{b})/2$, $\boldsymbol{t}_2 = (-\boldsymbol{a}+\boldsymbol{b})/2$ and $\boldsymbol{b}$. Since we can assumed that $b > a$, there are two cases:

(i) $b^2/3 \geq a^2$;

(ii) $b^2 > a^2 > b^2/3$.

The cells spanned by $\boldsymbol{t}_1$, $\boldsymbol{t}_2$ and $\boldsymbol{c}$ are reduced in the case (i), and numbered by 9. The cells spanned by $\boldsymbol{a}$, $\boldsymbol{t}_1$ and $\boldsymbol{c}$ are also reduced in the case (ii), and numbered by 10.

(3) Body-centered lattice

The ordinary centering vectors are denoted by $\boldsymbol{t}_1 = (-\boldsymbol{a}+\boldsymbol{b}+\boldsymbol{c})/2$, $\boldsymbol{t}_2 = (\boldsymbol{a}-\boldsymbol{b}+\boldsymbol{c})/2$ and $\boldsymbol{t}_3 = (\boldsymbol{a}+\boldsymbol{b}-\boldsymbol{c})/2$. The vector $\boldsymbol{t} = (\boldsymbol{a}+\boldsymbol{b}+\boldsymbol{c})/2$ is also the centering vector. All the lengths of the centering vectors are equal to one another, $t_1{}^2 = t_2{}^2 = t_3{}^2 = t^2 = (a^2+b^2+c^2)/4$.

When b^2 and c^2 are put to be xa^2 and ya^2, respectively, the following inequalities are obtained:

(1) $x > 1$ from $b > a$;

(2) $y > x$ from $c > b$;

(3) $x+y > 3$ from $t_1^2 > a^2$;

(4) $1+y > 3x$ from $t_1^2 > b^2$.

These inequalities can be solved graphically. The symbol ">" is replaced by "=" in order to draw lines. The region surrounded by the lines (2), (3) and (4) satisfies $a^2 < t^2$. The cell spanned by $\boldsymbol{a}$, $\boldsymbol{t}_1$ and $\boldsymbol{t}_2$ is reduced and numbered by 11. The region surrounded by the lines (1) and (4) satisfies $a^2 < b^2 < t^2$. The cell spanned by $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{t}$ is reduced and numbered by 12. The region surrounded by the lines (1), (2) and (3) satisfies $c^2 > b^2 > a^2 > t^2$. The cell spanned by $\boldsymbol{t}_1$, $\boldsymbol{t}_2$ and $\boldsymbol{t}_3$ is reduced and numbered by 13.

(4) **Face-centered lattice**

The three centering vectors are $\boldsymbol{t}_1 = (\boldsymbol{a}+\boldsymbol{b})/2$, $\boldsymbol{t}_2 = (\boldsymbol{b}+\boldsymbol{c})/2$ and $\boldsymbol{t}_3 = (\boldsymbol{c}+\boldsymbol{a})/2$. Two centering vectors are necessary to span this type of lattices. The absolute values of the basis vectors $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ are assumed to be $a < b < c$. The squares of the centering vectors satisfy $t_1^2 < t_3^2 < t_2^2$.

When $t_1^2 > a^2$, that is, $b^2/3 > a^2$, the cell spanned by $\boldsymbol{a}$, $\boldsymbol{t}_1$ and $\boldsymbol{t}_3$ is reduced. The cell is numbered by 14.

The cell spanned by $\boldsymbol{t}_1$, $\boldsymbol{t}_2$ and $\boldsymbol{t}_3$ is reducible. When $\boldsymbol{t}_1' = (-\boldsymbol{a}+\boldsymbol{b})/2$, the reduced cell is spanned by $\boldsymbol{t}_1'$, $\boldsymbol{t}_1$ and $\boldsymbol{t}_3$, and numbered by 15. Compare the cell with the face-centered cubic cell.

Tetragonal lattices

(1) **Primitive lattice**

The cells spanned by $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ are reduced, and numbered by 16.

(2) **Body-centered lattice**

The body-centering vectors are $\boldsymbol{t}_1 = (-\boldsymbol{a}+\boldsymbol{b}+\boldsymbol{c})/2$, $\boldsymbol{t}_2 = (\boldsymbol{a}-\boldsymbol{b}+\boldsymbol{c})/2$ and $\boldsymbol{t}_3 = (\boldsymbol{a}+\boldsymbol{b}-\boldsymbol{c})/2$, where $t_1^2 = t_2^2 = t_3^2 = (a^2+b^2+c^2)/4$. The vector $\boldsymbol{t} = (\boldsymbol{a}+\boldsymbol{b}+\boldsymbol{c})/2$ is also used as the centering vector.

If the centering vectors are longer than the length of $\boldsymbol{a}$, that is, $(2a^2+c^2)/4 > a^2$, hence $c^2 > 2a^2$, the cell spanned by $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{t}$ is reduced and numbered by 18.

The vector $\boldsymbol{c}$ becomes shorter than the centering vectors when $3c^2 > 2a^2$. Hence, when $2a^2 > c^2 > 2a^2/3$, the centering vectors are shorter than $\boldsymbol{a}$ and $\boldsymbol{c}$. The centering vectors become the basis vectors. The cell is numbered by 17. The cells of No. 6 and 7 in I. T. correspond to this cell.

When $2a^2/3 \geq c^2$, $\boldsymbol{c}$ becomes shorter than the centering vectors, so that $\boldsymbol{c}$ and the two centering vectors become the basis vectors. This cell is numbered by 19. This reduced cell should correspond to the No. 18 cell in I. T. The basis vectors of the No. 18 cell are $(\boldsymbol{a}+\boldsymbol{b}+2\boldsymbol{c})/3$, $(-\boldsymbol{a}-\boldsymbol{b}+\boldsymbol{c})/3$ and $(2\boldsymbol{a}-\boldsymbol{b}+\boldsymbol{c})/3$. The tensor elements obtained from these basis vectors contradict with those given in Table 9. 3. 1 of I. T. When $a^2 = 100$ and $c^2 = 40$, the tensor elements become $A = 40$, $B = 60$, $C = 60$, $D = 10$, $E = -20$ and $F = -20$ by the numerical calculation. These tensor elements accord with the values obtained from Table 1. Since this cell should be the type- I of I. T., the obtained elements do not contradict with those obtained from Table 9. 3. 1 of I. T..

Hexagonal lattice

The cells spanned by $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ are reduced, and numbered by 20.

Rhombohedral lattice

The lattice parameters of this lattice should be $a=b=c$ and $\alpha=\beta=\gamma$. When $1/2 \geq \cos\alpha > -1/2$, the results of addition and subtraction of any two basis vectors are equal to or longer than the basis vectors. Then, the two dimensional lattices spanned by the basis vectors $\boldsymbol{a}$, $\boldsymbol{b}$ or $\boldsymbol{c}$ are reduced. If $(\boldsymbol{a}+\boldsymbol{b}+\boldsymbol{c})^2 \geq c^2$, the value of $\cos\alpha$ should satisfy

$$\cos\alpha \geq -1/3 .$$

Hence, if

$$1/2 \geq \cos\alpha \geq -1/3,$$

the cell spanned by $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ are reduced. This cell is numbered by 21 and corresponds the cells of No. 2 and 4 in I. T..

When $-1/3 > \cos\alpha > -1/2$, then $(\boldsymbol{a}+\boldsymbol{b}+\boldsymbol{c})^2 < c^2$. Since $(\boldsymbol{a}+\boldsymbol{b})^2 > b^2$, the shortest vector in the lattice is $\boldsymbol{a}+\boldsymbol{b}+\boldsymbol{c}$. The cell spanned by $\boldsymbol{a}'=\boldsymbol{a}+\boldsymbol{b}+\boldsymbol{c}$, $\boldsymbol{b}'=\boldsymbol{a}$ and $\boldsymbol{c}'=\boldsymbol{b}$ is reduced and numbered by 22.

When $\cos\alpha > 1/2$, then $(\boldsymbol{a}\pm\boldsymbol{b})^2 < a^2$. The cell spanned by $\boldsymbol{a}'=\boldsymbol{a}$, $\boldsymbol{b}'=\boldsymbol{b}-\boldsymbol{a}$ and $\boldsymbol{c}'=\boldsymbol{c}-\boldsymbol{a}$ is reduced and numbered by 23.

Cubic lattices

The primitive and body-centered cells are reduced, the basis vectors are $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$, and $\boldsymbol{t}_1=(-\boldsymbol{a}+\boldsymbol{b}+\boldsymbol{c})/2$, $\boldsymbol{t}_2=(\boldsymbol{a}-\boldsymbol{b}+\boldsymbol{c})/2$ and $\boldsymbol{t}_3=(\boldsymbol{a}+\boldsymbol{b}-\boldsymbol{c})/2$, respectively.

Quite similarly to the face-centered orthorhombic lattice, the face-centered cell is reducible, and the reduced cell spanned by $\boldsymbol{t}_1=(\boldsymbol{a}+\boldsymbol{b})/2$, $\boldsymbol{t}_1'=(-\boldsymbol{a}+\boldsymbol{b})/2$ and $\boldsymbol{t}_2'=(-\boldsymbol{b}+\boldsymbol{c})/2$, accords with the result of the calculation. The basis vectors can be chosen many ways.

In summary, the contradicted results between the present study and the Tables 9. 3. 1 and 9. 3. 2 are the cells of No. 1, 18 and 43 except the difference due to the types. The basis of No.18 in I. T. indicated in Table 9. 3. 1 may be wrong.

The results of the examination of the 44 reduced cells in I. T. are listed in Table 1. The Numbers in the first column are the Number of the reduced cells proposed in this article. The Numbers of the second column are the Numbers of reduced cells in I. T.. The third column is for lattice symmetry. The fourth column is for the Bravais lattices of the reduced cells. The fifth column is for the basis vectors of the reduced cell. The basis vector $\boldsymbol{a}'$ is the shortest and $\boldsymbol{c}'$ is the longest. The sixth, seventh and eighth columns are for the elements of the metric tensors, $D=\boldsymbol{b}'\cdot\boldsymbol{c}'$, $E=\boldsymbol{c}'\cdot\boldsymbol{a}'$ and $F=\boldsymbol{a}'\cdot\boldsymbol{b}'$. The bases are set in accordance with the results of the calculations. The reduced cells in I. T. surrounded by horizontal lines are equivalent to one another.

Table 1

No.	I.T. No.	Lattice symmetry	Bravais type	Basis Vector a'	b'	c'	D	E	E
1	31 44	Triclinic	aP	a a	b b	c c	$b\cos\alpha$ $b\cos\alpha$	$ca\cos\beta$ $ca\cos\beta$	$ab\cos\gamma$ $ab\cos\gamma$
2	33 34 35	Monoclinic	mP	a a $-a$	b c a	c $-b$ c	0 0 $ca\cos\beta$	$ca\cos\beta$ 0 0	0 $ca\cos\beta$ 0
3	28 29 30	Monoclinic	mC	$-a$ $-a$ c	c t_1 a	t_1 c t_2	$ca\cos\beta/2$ $ca\cos\beta/2$ $-a^2/2$	$-a^2/2$ $-ca\cos\beta$ $ca\cos\beta/2$	$-ca\cos\beta$ $-a^2/2$ $-ca\cos\beta$
4	25 20	Monoclinic	mC	c c	t_1 t_1	t_2 t_2	$(b^2-a^2)/4$ $(b^2-a^2)/4$	$-ca\cos\beta/2$ $-ca\cos\beta/2$	$ca\cos\beta/2$ $ca\cos\beta/2$
4'	14 10	Monoclinic	mC	t_1 t_1	t_2 t_2	c c	$-ca\cos\beta/2$ $-ca\cos\beta/2$	$ca\cos\beta/2$ $ca\cos\beta/2$	$(b^2-a^2)/4$ $(b^2-a^2)/4$
5	17	Monoclinic	mC	t_1	t_2	$-c-t_1$	$-(a^2+b^2)/4$ $-ca\cos\beta/2$	$-(b^2-a^2)/4$ $+ca\cos\beta/2$	$(b^2-a^2)/4$
6	37 39 41	Monoclinic	mC	$-b$ $-b$ c	c t_1 $-b$	t_1 c t_1	$ca\cos\beta/2$ $ca\cos\beta/2$ $-b^2/2$	$-b^2/2$ 0 $ca\cos\beta/2$	0 $-b^2/2$ 0
7	27	Monoclinic	mC	$-b$	t_1	$c+t_1$	$(a^2+b^2)/4$ $+ca\cos\beta/2$	$-b^2/2$	$-b^2/2$
8	32	Orthorhombic	oP	a	b	c	0	0	0
9	13 23	Orthorhombic	oC	t_1 c	t_2 t_1	c t_2	0 $(b^2-a^2)/4$	0 0	$(b^2-a^2)/4$ 0
10	36 38 40	Orthorhombic	oC	$-a$ $-a$ c	c t_1 $-a$	t_1 c t_1	0 0 $-a^2/2$	$-a^2/2$ 0 0	0 $-a^2/2$ 0
11	8	Orthorhombic	oI	t_1	t_2	t_3	$(a^2-b^2-c^2)/4$	$-(a^2-c^2+b^2)/4$	$-(a^2-b^2+c^2)/4$
12	19	Orthorhombic	oI	a	t_1	$-t_3$	$(a^2-b^2+c^2)/4$	$-a^2/2$	$-a^2/2$
13	42	Orthorhombic	oI	a	b	$-t$	$-b^2/2$	$-a^2/2$	0
14	16	Orthorhombic	oF	t_1'	t_1	t_3	$-a^2/4$	$a^2/4$	$(b^2-a^2)/2$
15	26	Orthorhombic		$-a$	t_1	t_3	$a^2/4$	$-a^2/2$	$-a^2/2$
16	11 21	Tetragonal	tP	a c	b a	c b	0 0	0 0	0 0
17	6 7	Tetragonal	tI tI	t_1 t_1	t_2 t_2	t_3 t_3	$-c^2/4$ $-c^2/4$	$-c^2/4$ $-c^2/4$	$(-2a^2+c^2)/4$ $(-2a^2+c^2)/4$
18	15	Tetragonal	tI	a	b	$-t$	$-a^2/2$	$-a^2/2$	0
19	18?	Tetragonal	tI	$-c$	t_1	t	$c^2/4$	$-c^2/2$	$-c^2/2$
20	12 22	Hexagonal	hP	a c	b a	c b	0 $-a^2/2$	0 0	$-a^2/2$ 0
21	2 4	Rhombohedral	hR	a a	b b	c c	$a^2\cos\alpha$ $a^2\cos\alpha$	$a^2\cos\alpha$ $a^2\cos\alpha$	$a^2\cos\alpha$ $a^2\cos\alpha$
22	24	Rhombohedral	hR	$a+b+c$	a	b	$a^2\cos\alpha$	$a^2(1+Z\cos\alpha)$	$a^2(1+Z\cos\alpha)$
23	9	Rhombohedral	hR	a	$b-a$	$c-b$	$-a^2(1-\cos\alpha)$	0	$-a^2(1-\cos\alpha)$
24	3	Cubic	cP	a	b	c	0	0	0
25	5	Cubic	cI	t_1	t_2	t_3	$-a^2/4$	$-a^2/4$	$-a^2/4$
26	1	Cubic	cF	t_1	t_2'	t_1'	$-a^2/4$	0	$-a^2/4$