Ferroelectric Transformations of Tensorial Properties in Regular Ferroelectrics

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There are 19 kinds of regular ferroelectrics. Their tensorial properties are changed with their state transition in a manner unique and definite to each of the 19 kinds. A systematic investigation is made into this manner of change. The kinds of tensors examined are the polar and axial tensors of ranks two, three, and four. This theory is expected to serve not only for predicting the manners of change of the tensorial properties in the regular ferroelectrics, but also for determining the kind of a regular ferroelectric crystal and for judging regularity or irregularity of a ferroelectric crystal.

1. INTRODUCTION

In a previous paper[1] we have adopted as a most reasonable definition of ferroelectricity the following one: When a crystal plate, with certain Miller indices, of a crystal has two stable states of different polarizations at no electric field and can alternate between these states by means of a suitable alternating electric field, then the crystal plate or the crystal is said to be ferroelectric or to exhibit ferroelectricity; here the two stable states are assumed to be identical or enantiomorphous in crystal structure and to be equal in plate thickness. In this definition of ferroelectricity, in fact, the phrase "of different polarizations" is not necessary. For, if the state transition is possible by means of the electric field, it is natural that the two states should be different in polarization. (If the two states were equal in polarization, the electric field would not do any work at the state transition, which means impossibility of the state transition by the electric field.) The two stable states are usually at no stress.

From the above definition it is derived[1] that the ferroelectric crystal plate must be *normally polar* (see below), or that the ferroelectric crystal must belong to a noncentrosymmetrical group. It is also reasoned[1] that a crystal belonging to a noncentrosymmetrical but nonpolar group is scarcely expected to exhibit ferroelectricity. It is, however, not concluded[1] that *every* ferroelectric crystal must belong to a polar group. (No ferroelectrics have yet been discovered which belong to a nonpolar group.)

The term "being normally polar" has been defined in Ref. 1: A crystal plate is referred to as being normally nonpolar or normally polar, according to whether opposite senses of the normal to the crystal plate are equivalent in symmetry or not. It is obvious that the crystal plates of a crystal belonging to a centrosymmetrical group are all normally nonpolar, and that, conversely, if all crystal plates of a crystal are normally nonpolar, the crystal belongs to a centrosymmetrical group. Hence, for a crystal plate to be normally polar, its *parent* crystal must belong to a noncentrosymmetrical group; and any crystal belonging to a noncentrosymmetrical group necessarily has normally-polar crystal plates. It should not, however, be taken that all crystal plates of all noncentrosymmetrical crystals are normally polar.

In Ref. 1 we have introduced the concept of the *regular* ferroelectric crystals: A ferroelectric crystal is said to be regular when (1) in any crystal plate with any Miller indices of the crystal the space lattice in one of the two stable states is parallel to that in the other state and (2) the notion of the two stable states is possible not only for the individual crystal plates but for the crystal as a whole. From this definition it is derived[1] that a regular ferroelectric crystal must belong to a polar group. Hence, it also follows that a ferroelectric crystal belonging to a nonpolar group, if any, must be irregular. A ferroelectric crystal belonging to a polar group is regular if it only satisfies the first condition for regularity; for in this case it satisfies also the second condition. Many of the ferroelectric crystals discovered up to now are considered to be regular. As an example of irregular ferroelectric crystal, there is Rochelle salt; as is well known, in the crystal plate normal to the polar axis of this crystal the space lattice is not kept parallel at the state transition.

For the regular ferroelectrics, there are three types of state transition, viz., inversion, reflection, and rotation types.[1] The regular ferroelectrics are divisible into 19 kinds in accordance with their point group, Bravais lattice, and type of state transition.[1] (What has so far been stated is all given also in Ref. 1, but in a full account. One who wants to know the details is recommended to see Ref. 1.)

In Ref. 1 it has been suggested that when the regular ferroelectrics undergo the state transition, their tensorial properties are changed in a manner unique and definite to each of the 19 kinds. In this paper, a systematic investigation is made into this manner of change (see Sec. 3). The kinds of tensors examined are the polar and axial tensors of ranks two, three, and four. The polar tensor of rank two and the axial tensor of rank two need not be symmetric. But the polar tensor of rank three and the axial tensor of rank three are assumed to be partially symmetric, i.e., to be such that their (i,j,k) element T_{ijk} is equal to their (i,k,j) element T_{ikj}. (The tensor in which $T_{ijk}=T_{jik}$ can be translated into the tensor in which $T_{ijk}=T_{ikj}$. The completely symmetric tensor, in which $T_{ijk}=T_{ikj}=T_{jik}$, is regarded as

[1] K. Aizu, Revs. Mod. Phys. 34, 550 (1962).

a special case of the tensor in which $T_{ijk}=T_{ikj}$.) The polar tensor of rank four and the axial tensor of rank four are also assumed to be partially symmetric, i.e., to be such that $T_{ijkl}=T_{jikl}=T_{ijlk}$. (The completely symmetric tensor, in which $T_{ijkl}=T_{jikl}=T_{ijlk}=T_{klij}$, is regarded as a special case of the above tensor.)

As examples of these tensors, there are the dielectric-susceptibility tensor (a symmetric polar tensor of rank two), the gyration tensor[2] (a symmetric axial tensor of rank two), the piezoelectric-modulus tensor (a partially-symmetric polar tensor of rank three), the "electro-gyration" tensor (a partially-symmetric axial tensor of rank three), the elastic-coefficient tensor (a completely-symmetric polar tensor of rank four), and the "piezo-gyration" tensor (a partially-symmetric axial tensor of rank four). Here, the "electrogyration" tensor means the tensor equal to the rate of change of the gyration tensor with the electric-field vector at zero value of the electric-field vector. The "piezogyration" tensor means the tensor equal to the rate of change of the gyration tensor with the stress tensor at zero value of the stress tensor.

The present theory is expected to serve not only for predicting the manners of change of the tensorial properties in the regular ferroelectrics, but also for determining the kind of a regular ferroelectric crystal and for judging regularity or irregularity of a ferroelectric crystal. We explain the latter uses below.

The regular ferroelectrics belonging to the point group 4, 6, 3, or 3*m* are divided into two or more kinds.[1] When the point group of a regular ferroelectric crystal is known, for example, to be 4, there are a few methods to find which kind, *r*4-I or *r*4-II (see Sec. 2), the crystal belongs to. The present theory furnishes one method. It consists in that the manner of change of a suitable tensorial property of the crystal with the state transition is observed experimentally and compared with the predictions of the present theory.

If a tensorial property of a ferroelectric crystal is changed with the state transition in a different manner than is predicted by the present theory, it is concluded that this ferroelectric crystal must be irregular. If one or a few tensorial properties of a ferroelectric crystal are changed with the state transition in exactly the same manner as predicted by the present theory, this ferroelectric crystal is expected to be regular.

It may be convenient to assign a symbol to each of the 19 kinds of regular ferroelectrics. We first undertake this, in next section, before proceeding to the principal subject.

2. NEW NOTATIONS FOR THE 19 KINDS OF REGULAR FERROELECTRICS

Each of the point groups 1, *m*, 2, *mm*2, 4*mm*, and 6*mm* comprises only one kind.[1] We agree to denote these six kinds by

$$r1,\quad rm,\quad r2,\quad rmm2,\quad r4mm,\quad r6mm. \qquad \text{(a)}$$

(The prefix "*r*" means "regular." We shall use the prefix "*i*" for the kinds of irregular ferroelectrics.) The kind *r*1 is of inversion type.[1] The kind *rm* is of inversion type and also of rotation type.[1] The kind *r*2 is of inversion type and of reflection type.[1] The kind *rmm*2 is simultaneously of inversion type, of reflection type, and of rotation type. The kinds *r*4*mm* and *r*6*mm* are also simultaneously of inversion type, of reflection type, and of rotation type.

Each of the point groups 4 and 6 comprises two kinds[1]; we agree to denote these four kinds by

$$r4\text{-I},\quad r4\text{-II},\quad r6\text{-I},\quad r6\text{-II}. \qquad \text{(b)}$$

The kinds *r*4-I and *r*6-I are of inversion type as well as of reflection type[1]; the kinds *r*4-II and *r*6-II are of rotation type.[1]

In the trigonal system, as is well known, there are two kinds of Bravais lattices, viz., trigonal *R* and hexagonal *P*. The point group 3 having the trigonal *R* lattice comprises two kinds and the point group 3*m* having the trigonal *R* lattice comprises only one kind.[1] We denote these by

$$r3R\text{-I},\quad r3R\text{-II},\quad r3mR. \qquad \text{(c)}$$

The kind *r*3*R*-I is of inversion type and the kind *r*3*R*-II is of rotation type. The kind *r*3*mR* is of inversion type as well as of rotation type.

The point group 3 having the hexagonal *P* lattice comprises four kinds,[1] which we denote by

$$r3P\text{-I},\quad r3P\text{-II},\quad r3P\text{-III},\quad r3P\text{-IV}. \qquad \text{(d)}$$

The first kind is of inversion type, the second of reflection type, the third of rotation type, and the fourth of rotation type.

The point group 3*m* having the hexagonal *P* lattice comprises two kinds,[1] which are denoted by

$$r3mP\text{-I},\quad r3mP\text{-II}. \qquad \text{(e)}$$

The first kind is of inversion type and of rotation type; the second kind is of reflection type and of rotation type. Now it is noticed that the symbols appearing in (a) to (e) count 19.

3. FERROELECTRIC TRANSFORMATIONS OF TENSORIAL PROPERTIES

3.1. Preliminary Remarks

A tensor is usually represented in terms of a matrix. The dimensions of this matrix are, however, not unique. For example, a partially symmetric tensor of rank three may be represented in terms of three 3×3 symmetric matrices or one 3×6 matrix or one 1×18 matrix. From the theoretical point of view, the first manner of representation is often the most convenient and the third is

[2] See, for example, J. F. Nye, *Physical Properties of Crystals* (Clarendon Press, Oxford, England, 1957).

often the least convenient. For a compact printing, however, the third manner is the most convenient and the first is the least convenient. Actually, it seems that the second manner is the most frequently used.

In the following subsections we represent a tensor of rank two in terms of a 3×3 matrix, a partially-symmetric tensor of rank three in terms of a 3×6 matrix, and a partially-symmetric tensor of rank four in terms of a 6×6 matrix. For this purpose we replace a commutable double suffix by a single suffix:

$$11\rightarrow 1,\quad 22\rightarrow 2,\quad 33\rightarrow 3,\quad 23 \text{ and } 32\rightarrow 4,$$
$$31 \text{ and } 13\rightarrow 5,\quad 12 \text{ and } 21\rightarrow 6.$$

Thus, in a partially-symmetric tensor of rank three, for example the (1,4) element of its matrix T_{14} corresponds to T_{123} or T_{132}; in a partially-symmetric tensor of rank four, for example the (4,5) element of its matrix T_{45} corresponds to T_{2331}, T_{3231}, T_{2313}, or T_{3213}.

Although a tensor is independent of the choice of the Cartesian-coordinate axes, its matrix is not so. Until the x, y, and z axes are fixed, the matrix cannot be determined. In the following subsections the x, y, z axes are taken common to the two stable states of the ferroelectrics; or in other words, the x, y, z axes are spatially fixed and independent of the state transition. In all kinds except *r*1, *rm*, and *r*2, the unique axis is taken as the z axis. In the kinds *rm* and *r*2, the unique axis is taken as either the z or the y axis; the former setting is referred to as the first setting, and the latter as the second. In the kinds *rmm*2, *r*4*mm*, and *r*6*mm*, each of the x and y axes is taken normal to one of the mirror planes of symmetry. In the kinds *r*3*mR*, *r*3*mP*-I, and *r*3*mP*-II, either the x or the y axis is taken normal to one of the mirror planes of symmetry. In the kind *r*1, the x, y, z axes are arbitrarily taken. There is a case that the value of every element of a matrix is independent of the choice of the x axis (as long as the x axis is at a right angle to the z axis). In this case we say simply "The direction of the x axis is free."

The matrices appearing in Subsec. 3.2 are numbered as (2P:1), (2P:2), (2P:3), etc. The matrices appearing in Subsec. 3.3 are numbered as (2A:1), (2A:2), (2A:3), etc. "2P" is used for signification of the "polar" tensor of rank "two," and "2A" for signification of the "axial" tensor of rank "two." The matrices appearing in other subsections are similarly numbered. The phrase "the state transition" is abbreviated "S.T."

In the following subsections, no method of proof is stated; only the results are shown. We here illustrate the method of proof by a consideration of the case of the partially symmetric polar tensor of rank three and the kinds *r*4-I and *r*4-II (see Subsec. 3.4). In the point group 4, and hence in the kinds *r*4-I and *r*4-II, as is well known, the partially symmetric tensor of rank three has a form of (3P:7) when the z axis is taken parallel to the tetragonal unique axis. The value of every element of this matrix is independent of the choice of the x axis. The kind *r*4-I is of inversion type and also of reflection type; one of its two stable states is obtained by performing upon the other the inversion operation or the reflection operation across the plane normal to the tetragonal unique axis.[1] The tensor (3P:7) is changed to the tensor (3P:8) by either of the above two operations. (It should be noted that the x, y, z axes are spatially fixed and independent of those operations.) In the kind *r*4-I, therefore, it is concluded that the tensor (3P:7) in one state is changed to the tensor (3P:8) by the state transition. The kind *r*4-II is of rotation type; one of its two stable states is obtained by performing upon the other a 180° rotation operation about an axis that is both perpendicular to the tetragonal unique axis and at 90° or 45° to one of the side faces of the unit-cell tetragonal prism.[1] The tensor (3P:7) is changed to the tensor (3P:9) by the above operation. In the kind *r*4-II, therefore, it is concluded that the tensor (3P:7) in one state is changed to the tensor (3P:9) by the state transition.

It is to be emphasized that the present paper is the first to determine systematically not the matrices of the tensorial properties in one state, but the change of the tensorial properties with the state transition, for each of the 19 kinds of regular ferroelectrics.

3.2. Polar Tensor of Rank Two

In the kind *r*1, the tensor in one state is

$$\begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix}. \qquad (2P{:}1)$$

This is unchanged by S.T.

In the kind *rm*, the tensor in one state is

$$\begin{pmatrix} T_{11} & T_{12} & 0 \\ T_{21} & T_{22} & 0 \\ 0 & 0 & T_{33} \end{pmatrix} \qquad (2P{:}2)$$

in the first setting, and

$$\begin{pmatrix} T_{11} & 0 & T_{13} \\ 0 & T_{22} & 0 \\ T_{31} & 0 & T_{33} \end{pmatrix} \qquad (2P{:}3)$$

in the second setting. This tensor is unchanged by S.T.

In the kind *r*2, the tensor in one state is (2P:2) in the first setting and (2P:3) in the second setting. This is unchanged by S.T.

In the kind *rmm*2, the tensor in one state is

$$\begin{pmatrix} T_{11} & 0 & 0 \\ 0 & T_{22} & 0 \\ 0 & 0 & T_{33} \end{pmatrix}. \qquad (2P{:}4)$$

This is unchanged by S.T.

In the kinds *r*4-I and *r*4-II, the tensor in one state is

$$\begin{pmatrix} a & c & 0 \\ -c & a & 0 \\ 0 & 0 & b \end{pmatrix}. \qquad (2P{:}5)$$

(The direction of the x axis is free.) By S.T. this is unchanged for $r4$-I and changed for $r4$-II to

$$\begin{bmatrix} a & -c & 0 \\ c & a & 0 \\ 0 & 0 & b \end{bmatrix}. \tag{2P:6}$$

In the kind $r4mm$, the tensor in one state is

$$\begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & b \end{bmatrix}. \tag{2P:7}$$

(The direction of the x axis is free.) This is unchanged by S.T.

In the kinds $r6$-I and $r6$-II, the tensor in one state is (2P:5). By S.T. this is unchanged for $r6$-I and changed for $r6$-II to (2P:6). In the kind $r6mm$, the tensor in one state is (2P:7). This is unchanged by S.T.

In the kinds $r3R$-I and $r3R$-II, the tensor in one state is (2P:5). By S.T. this is unchanged for $r3R$-I and changed for $r3R$-II to (2P:6). In the kind $r3mR$, the tensor in one state is (2P:7). This is unchanged by S.T.

In the kinds $r3P$'s, the tensor in one state is (2P:5). By S.T. this is unchanged for $r3P$-I and $r3P$-II, and changed for $r3P$-III and $r3P$-IV to (2P:6). In the kinds $r3mP$'s, the tensor in one state is (2P:7). By S.T. this is unchanged for both $r3mP$-I and $r3mP$-II.

3.3. Axial Tensor of Rank Two

In the kind $r1$, the tensor in one state is

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix}. \tag{2A:1}$$

This is reversed in sign by S.T.

In the kind rm, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & T_{13} \\ 0 & 0 & T_{23} \\ T_{31} & T_{32} & 0 \end{bmatrix} \tag{2A:2}$$

in the first setting, and

$$\begin{bmatrix} 0 & T_{12} & 0 \\ T_{21} & 0 & T_{23} \\ 0 & T_{32} & 0 \end{bmatrix} \tag{2A:3}$$

in the second setting. This tensor is reversed in sign by S.T.

In the kind $r2$, the tensor in one state is

$$\begin{bmatrix} T_{11} & T_{12} & 0 \\ T_{21} & T_{22} & 0 \\ 0 & 0 & T_{33} \end{bmatrix} \tag{2A:4}$$

in the first setting and

$$\begin{bmatrix} T_{11} & 0 & T_{13} \\ 0 & T_{22} & 0 \\ T_{31} & 0 & T_{33} \end{bmatrix} \tag{2A:5}$$

in the second setting. This tensor is reversed in sign by S.T.

In the kind $rmm2$, the tensor in one state is

$$\begin{bmatrix} 0 & T_{12} & 0 \\ T_{21} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{2A:6}$$

This is reversed in sign by S.T.

In the kinds $r4$-I and $r4$-II, the tensor in one state is

$$\begin{bmatrix} a & c & 0 \\ -c & a & 0 \\ 0 & 0 & b \end{bmatrix}. \tag{2A:7}$$

(The direction of the x axis is free.) By S.T. this is changed for $r4$-I to the tensor of opposite sign, i.e.,

$$\begin{bmatrix} -a & -c & 0 \\ c & -a & 0 \\ 0 & 0 & -b \end{bmatrix}, \tag{2A:8}$$

and for $r4$-II to

$$\begin{bmatrix} a & -c & 0 \\ c & a & 0 \\ 0 & 0 & b \end{bmatrix}. \tag{2A:9}$$

In the kind $r4mm$, the tensor in one state is

$$\begin{bmatrix} 0 & c & 0 \\ -c & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{2A:10}$$

(The direction of the x axis is free.) This is reversed in sign by S.T.

In the kinds $r6$-I and $r6$-II, the tensor in one state is (2A:7). By S.T. this is changed for $r6$-I to (2A:8) and for $r6$-II to (2A:9). In the kind $r6mm$, the tensor in one state is (2A:10). This is reversed in sign by S.T.

In the kinds $r3R$-I and $r3R$-II, the tensor in one state is (2A:7). By S.T. this is changed for $r3R$-I to (2A:8) and for $r3R$-II to (2A:9). In the kind $r3mR$, the tensor in one state is (2A:10). This is reversed in sign by S.T.

In the kinds $r3P$'s, the tensor in one state is (2A:7). By S.T. this is changed for $r3P$-I and $r3P$-II to (2A:8) and for $r3P$-III and $r3P$-IV to (2A:9). In the kinds $r3mP$'s, the tensor in one state is (2A:10). By S.T. this is reversed in sign for both $r3mP$-I and $r3mP$-II.

3.4. Polar Tensor of Rank Three

In the kind $r1$, the tensor in one state is

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} & T_{14} & T_{15} & T_{16} \\ T_{21} & T_{22} & T_{23} & T_{24} & T_{25} & T_{26} \\ T_{31} & T_{32} & T_{33} & T_{34} & T_{35} & T_{36} \end{bmatrix}. \tag{3P:1}$$

This is reversed in sign by S.T.

In the kind rm, the tensor in one state is

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} & 0 & 0 & T_{16} \\ T_{21} & T_{22} & T_{23} & 0 & 0 & T_{26} \\ 0 & 0 & 0 & T_{34} & T_{35} & 0 \end{bmatrix} \tag{3P:2}$$

in the first setting, and

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} & 0 & T_{15} & 0 \\ 0 & 0 & 0 & T_{24} & 0 & T_{26} \\ T_{31} & T_{32} & T_{33} & 0 & T_{35} & 0 \end{bmatrix} \qquad (3P:3)$$

in the second setting. This tensor is reversed in sign by S.T.

In the kind $r2$, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & T_{14} & T_{15} & 0 \\ 0 & 0 & 0 & T_{24} & T_{25} & 0 \\ T_{31} & T_{32} & T_{33} & 0 & 0 & T_{36} \end{bmatrix} \qquad (3P:4)$$

in the first setting, and

$$\begin{bmatrix} 0 & 0 & 0 & T_{14} & 0 & T_{16} \\ T_{21} & T_{22} & T_{23} & 0 & T_{25} & 0 \\ 0 & 0 & 0 & T_{34} & 0 & T_{36} \end{bmatrix} \qquad (3P:5)$$

in the second setting. This tensor is reversed in sign by S.T.

In the kind $rmm2$, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & 0 & T_{15} & 0 \\ 0 & 0 & 0 & T_{24} & 0 & 0 \\ T_{31} & T_{32} & T_{33} & 0 & 0 & 0 \end{bmatrix}. \qquad (3P:6)$$

This is reversed in sign by S.T.

In the kinds $r4$-I and $r4$-II, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & d & c & 0 \\ 0 & 0 & 0 & c & -d & 0 \\ b & b & a & 0 & 0 & 0 \end{bmatrix}. \qquad (3P:7)$$

(The direction of the x axis is free.) By S.T. this is changed for $r4$-I to the tensor of opposite sign, i.e.,

$$\begin{bmatrix} 0 & 0 & 0 & -d & -c & 0 \\ 0 & 0 & 0 & -c & d & 0 \\ -b & -b & -a & 0 & 0 & 0 \end{bmatrix}, \qquad (3P:8)$$

and for $r4$-II to

$$\begin{bmatrix} 0 & 0 & 0 & d & -c & 0 \\ 0 & 0 & 0 & -c & -d & 0 \\ -b & -b & -a & 0 & 0 & 0 \end{bmatrix}. \qquad (3P:9)$$

In the kind $r4mm$, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & 0 & c & 0 \\ 0 & 0 & 0 & c & 0 & 0 \\ b & b & a & 0 & 0 & 0 \end{bmatrix}. \qquad (3P:10)$$

(The direction of the x axis is free.) This is reversed in sign by S.T.

In the kinds $r6$-I and $r6$-II, the tensor in one state is (3P:7). By S.T. this is changed for $r6$-I to (3P:8) and for $r6$-II to (3P:9). In the kind $r6mm$, the tensor in one state is (3P:10). This is reversed in sign by S.T.

In the kinds $r3R$-I and $r3R$-II, the tensor in one state is

$$\begin{bmatrix} -e & e & 0 & d & c & f \\ f & -f & 0 & c & -d & e \\ b & b & a & 0 & 0 & 0 \end{bmatrix}. \qquad (3P:11)$$

For $r3R$-I, this is changed by S.T. to the tensor of opposite sign, i.e.,

$$\begin{bmatrix} e & -e & 0 & -d & -c & -f \\ -f & f & 0 & -c & d & -e \\ -b & -b & -a & 0 & 0 & 0 \end{bmatrix}. \qquad (3P:12)$$

For $r3R$-II, if the x axis is taken normal to both the trigonal unique axis and one of the edges of the unit-cell rhombohedron, the tensor (3P:11) is changed by S.T. to

$$\begin{bmatrix} -e & e & 0 & d & -c & -f \\ -f & f & 0 & -c & -d & e \\ -b & -b & -a & 0 & 0 & 0 \end{bmatrix}; \qquad (3P:13)$$

if the y axis is taken normal to both the trigonal unique axis and one of the edges of the rhombohedron, the tensor (3P:11) is changed to

$$\begin{bmatrix} e & -e & 0 & d & -c & f \\ f & -f & 0 & -c & -d & -e \\ -b & -b & -a & 0 & 0 & 0 \end{bmatrix}. \qquad (3P:14)$$

In the kind $r3mR$, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & 0 & c & f \\ f & -f & 0 & c & 0 & 0 \\ b & b & a & 0 & 0 & 0 \end{bmatrix} \qquad (3P:15)$$

or

$$\begin{bmatrix} -e & e & 0 & 0 & c & 0 \\ 0 & 0 & 0 & c & 0 & e \\ b & b & a & 0 & 0 & 0 \end{bmatrix} \qquad (3P:16)$$

according as to which axis, x or y, is taken normal to one of the mirror planes of symmetry. By S.T. the tensor (3P:15) or (3P:16) is reversed in sign.

In the kinds $r3P$'s, the tensor in one state is (3P:11). By S.T. this is changed for $r3P$-I to (3P:12) and for $r3P$-II to

$$\begin{bmatrix} -e & e & 0 & -d & -c & f \\ f & -f & 0 & -c & d & e \\ -b & -b & -a & 0 & 0 & 0 \end{bmatrix}. \qquad (3P:17)$$

If the x axis is taken normal to one of the side faces of the unit-cell hexagonal prism, then by S.T. the tensor (3P:11) is changed for $r3P$-III to (3P:13) and for $r3P$-IV to (3P:14); if the y axis is taken normal to one of the side faces of the hexagonal prism, the tensor (3P:11) is changed for $r3P$-III to (3P:14) and for $r3P$-IV to (3P:13).

In the kinds $r3mP$-I and $r3mP$-II, if the x axis is taken normal to one of the mirror planes of symmetry, the tensor in one state is (3P:15). By S.T. this is changed for $r3mP$-I to the tensor in opposite sign, i.e.,

$$\begin{bmatrix} 0 & 0 & 0 & 0 & -c & -f \\ -f & f & 0 & -c & 0 & 0 \\ -b & -b & -a & 0 & 0 & 0 \end{bmatrix} \qquad (3P:18)$$

and for $r3mP$-II to

$$\begin{bmatrix} 0 & 0 & 0 & 0 & -c & f \\ f & -f & 0 & -c & 0 & 0 \\ -b & -b & -a & 0 & 0 & 0 \end{bmatrix}. \quad \text{(3P:19)}$$

If the y axis is taken normal to one of the mirror planes of symmetry, the tensor in one state is (3P:16). By S.T. this is changed for $r3mP$-I to the tensor of opposite sign, i.e.,

$$\begin{bmatrix} e & -e & 0 & 0 & -c & 0 \\ 0 & 0 & 0 & -c & 0 & -e \\ -b & -b & -a & 0 & 0 & 0 \end{bmatrix} \quad \text{(3P:20)}$$

and for $r3mP$-II to

$$\begin{bmatrix} -e & e & 0 & 0 & -c & 0 \\ 0 & 0 & 0 & -c & 0 & e \\ -b & -b & -a & 0 & 0 & 0 \end{bmatrix}. \quad \text{(3P:21)}$$

3.5. Axial Tensor of Rank Three

In the kind $r1$, the tensor in one state is

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} & T_{14} & T_{15} & T_{16} \\ T_{21} & T_{22} & T_{23} & T_{24} & T_{25} & T_{26} \\ T_{31} & T_{32} & T_{33} & T_{34} & T_{35} & T_{36} \end{bmatrix}. \quad \text{(3A:1)}$$

This is unchanged by S.T.

In the kind rm, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & T_{14} & T_{15} & 0 \\ 0 & 0 & 0 & T_{24} & T_{25} & 0 \\ T_{31} & T_{32} & T_{33} & 0 & 0 & T_{36} \end{bmatrix} \quad \text{(3A:2)}$$

in the first setting and

$$\begin{bmatrix} 0 & 0 & 0 & T_{14} & 0 & T_{16} \\ T_{21} & T_{22} & T_{23} & 0 & T_{25} & 0 \\ 0 & 0 & 0 & T_{34} & 0 & T_{36} \end{bmatrix} \quad \text{(3A:3)}$$

in the second setting. This tensor is unchanged by S.T.

In the kind $r2$, the tensor in one state is (3A:2) in the first setting and (3A:3) in the second setting. This is unchanged by S.T.

In the kind $rmm2$, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & T_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & T_{25} & 0 \\ 0 & 0 & 0 & 0 & 0 & T_{36} \end{bmatrix}. \quad \text{(3A:4)}$$

This is unchanged by S.T.

In the kinds $r4$-I and $r4$-II, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & a & b & 0 \\ 0 & 0 & 0 & b & -a & 0 \\ c & c & d & 0 & 0 & 0 \end{bmatrix}. \quad \text{(3A:5)}$$

(The direction of the x axis is free.) By S.T. this is unchanged for $r4$-I and changed for $r4$-II to

$$\begin{bmatrix} 0 & 0 & 0 & a & -b & 0 \\ 0 & 0 & 0 & -b & -a & 0 \\ -c & -c & -d & 0 & 0 & 0 \end{bmatrix}. \quad \text{(3A:6)}$$

In the kind $r4mm$, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & a & 0 & 0 \\ 0 & 0 & 0 & 0 & -a & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \quad \text{(3A:7)}$$

(The direction of the x axis is free.) This is unchanged by S.T.

In the kinds $r6$-I and $r6$-II, the tensor in one state is (3A:5). By S.T. this is unchanged for $r6$-I and changed for $r6$-II to (3A:6). In the kind $r6mm$, the tensor in one state is (3A:7). This is unchanged by S.T.

In the kinds $r3R$-I and $r3R$-II, the tensor in one state is

$$\begin{bmatrix} -e & e & 0 & a & b & f \\ f & -f & 0 & b & -a & e \\ c & c & d & 0 & 0 & 0 \end{bmatrix}. \quad \text{(3A:8)}$$

For $r3R$-I, this is unchanged by S.T. For $r3R$-II, if the x axis is taken normal to both the trigonal unique axis and one of the edges of the unit-cell rhombohedron, the tensor (3A:8) is changed by S.T. to

$$\begin{bmatrix} -e & e & 0 & a & -b & -f \\ -f & f & 0 & -b & -a & e \\ -c & -c & -d & 0 & 0 & 0 \end{bmatrix}; \quad \text{(3A:9)}$$

if the y axis is taken normal to both the trigonal unique axis and one of the edges of the rhombohedron, the tensor (3A:8) is changed to

$$\begin{bmatrix} e & -e & 0 & a & -b & f \\ f & -f & 0 & -b & -a & -e \\ -c & -c & -d & 0 & 0 & 0 \end{bmatrix}. \quad \text{(3A:10)}$$

In the kind $r3mR$, the tensor in one state is

$$\begin{bmatrix} -e & e & 0 & a & 0 & 0 \\ 0 & 0 & 0 & 0 & -a & e \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad \text{(3A:11)}$$

or

$$\begin{bmatrix} 0 & 0 & 0 & a & 0 & f \\ f & -f & 0 & 0 & -a & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad \text{(3A:12)}$$

according as to which axis, x or y, is taken normal to one of the mirror planes of symmetry. By S.T. the tensor (3A:11) or (3A:12) is unchanged.

In the kinds $r3P$'s, the tensor in one state is (3A:8). By S.T. this is unchanged for $r3P$-I and changed for $r3P$-II to

$$\begin{bmatrix} e & -e & 0 & a & b & -f \\ -f & f & 0 & b & -a & -e \\ c & c & d & 0 & 0 & 0 \end{bmatrix}. \quad \text{(3A:13)}$$

If the x axis is taken normal to one of the side faces of the unit-cell hexagonal prism, then by S.T. the tensor (3A:8) is changed for $r3P$-III to (3A:9) and for $r3P$-IV to (3A:10); if the y axis is taken normal to one of the side faces of the hexagonal prism, the tensor (3A:8) is changed for $r3P$-III to (3A:10) and for $r3P$-IV to (3A:9).

In the kinds $r3mP$-I and $r3mP$-II, if the x axis is taken normal to one of the mirror planes of symmetry, the tensor in one state is (3A:11). By S.T. this is unchanged for $r3mP$-I and changed for $r3mP$-II to

$$\begin{bmatrix} e & -e & 0 & a & 0 & 0 \\ 0 & 0 & 0 & 0 & -a & -e \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \quad (3A{:}14)$$

If the y axis is taken normal to one of the mirror planes of symmetry, the tensor in one state is (3A:12). By S.T. this is unchanged for $r3mP$-I and changed for $r3mP$-II to

$$\begin{bmatrix} 0 & 0 & 0 & a & 0 & -f \\ -f & f & 0 & 0 & -a & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \quad (3A{:}15)$$

3.6. Polar Tensor of Rank Four

In the kind $r1$, the tensor in one state comprises 36 independent elements. This tensor is unchanged by S.T.

In the kinds rm and $r2$, the tensor in one state is

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} & 0 & 0 & T_{16} \\ T_{21} & T_{22} & T_{23} & 0 & 0 & T_{26} \\ T_{31} & T_{32} & T_{33} & 0 & 0 & T_{36} \\ 0 & 0 & 0 & T_{44} & T_{45} & 0 \\ 0 & 0 & 0 & T_{54} & T_{55} & 0 \\ T_{61} & T_{62} & T_{63} & 0 & 0 & T_{66} \end{bmatrix} \quad (4P{:}1)$$

in the first setting, and

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} & 0 & T_{15} & 0 \\ T_{21} & T_{22} & T_{23} & 0 & T_{25} & 0 \\ T_{31} & T_{32} & T_{33} & 0 & T_{35} & 0 \\ 0 & 0 & 0 & T_{44} & 0 & T_{46} \\ T_{51} & T_{52} & T_{53} & 0 & T_{55} & 0 \\ 0 & 0 & 0 & T_{64} & 0 & T_{66} \end{bmatrix} \quad (4P{:}2)$$

in the second setting. This tensor is unchanged by S.T.

In the kind $rmm2$, the tensor in one state is

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} & 0 & 0 & 0 \\ T_{21} & T_{22} & T_{23} & 0 & 0 & 0 \\ T_{31} & T_{32} & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & T_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & T_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & T_{66} \end{bmatrix}. \quad (4P{:}3)$$

This is unchanged by S.T.

In the kinds $r4$-I and $r4$-II, the tensor in one state is

$$\begin{bmatrix} a & b & c & 0 & 0 & f \\ b & a & c & 0 & 0 & -f \\ d & d & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & e & h & 0 \\ 0 & 0 & 0 & -h & e & 0 \\ g & -g & 0 & 0 & 0 & T_{66} \end{bmatrix}. \quad (4P{:}4)$$

By S.T. this is unchanged for $r4$-I. For $r4$-II, if the x axis is taken normal or at 45° to one of the side faces of the unit-cell tetragonal prism, the tensor (4P:4) is changed by S.T. to

$$\begin{bmatrix} a & b & c & 0 & 0 & -f \\ b & a & c & 0 & 0 & f \\ d & d & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & e & -h & 0 \\ 0 & 0 & 0 & h & e & 0 \\ -g & g & 0 & 0 & 0 & T_{66} \end{bmatrix}. \quad (4P{:}5)$$

In the kind $r4mm$, the tensor in one state is

$$\begin{bmatrix} a & b & c & 0 & 0 & 0 \\ b & a & c & 0 & 0 & 0 \\ d & d & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & e & 0 & 0 \\ 0 & 0 & 0 & 0 & e & 0 \\ 0 & 0 & 0 & 0 & 0 & T_{66} \end{bmatrix}. \quad (4P{:}6)$$

This is unchanged by S.T.

In the kinds $r6$-I and $r6$-II, the tensor in one state is

$$\begin{bmatrix} a & b & c & 0 & 0 & f \\ b & a & c & 0 & 0 & -f \\ d & d & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & e & h & 0 \\ 0 & 0 & 0 & -h & e & 0 \\ -f & f & 0 & 0 & 0 & A \end{bmatrix}, \quad (4P{:}7)$$

where $A=\frac{1}{2}(a-b)$. (The direction of the x axis is free.) By S.T. this is unchanged for $r6$-I and changed for $r6$-II to

$$\begin{bmatrix} a & b & c & 0 & 0 & -f \\ b & a & c & 0 & 0 & f \\ d & d & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & e & -h & 0 \\ 0 & 0 & 0 & h & e & 0 \\ f & -f & 0 & 0 & 0 & A \end{bmatrix}. \quad (4P{:}8)$$

In the kind $r6mm$, the tensor in one state is

$$\begin{bmatrix} a & b & c & 0 & 0 & 0 \\ b & a & c & 0 & 0 & 0 \\ d & d & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & e & 0 & 0 \\ 0 & 0 & 0 & 0 & e & 0 \\ 0 & 0 & 0 & 0 & 0 & A \end{bmatrix}, \quad (4P{:}9)$$

where $A=\frac{1}{2}(a-b)$. (The direction of the x axis is free.) This is unchanged by S.T.

In the kinds $r3R$-I and $r3R$-II, the tensor in one state is

$$\begin{bmatrix} a & b & c & k & -m & f \\ b & a & c & -k & m & -f \\ d & d & T_{33} & 0 & 0 & 0 \\ l & -l & 0 & e & h & n \\ -n & n & 0 & -h & e & l \\ -f & f & 0 & m & k & A \end{bmatrix}, \quad (4P{:}10)$$

where $A=\frac{1}{2}(a-b)$. For $r3R$-I, this is unchanged by S.T. For $r3R$-II, if the x axis is taken normal to one of the edges of the unit-cell rhombohedron, the tensor (4P:10) is changed by S.T. to

$$\begin{bmatrix} a & b & c & k & m & -f \\ b & a & c & -k & -m & f \\ d & d & T_{33} & 0 & 0 & 0 \\ l & -l & 0 & e & -h & -n \\ n & -n & 0 & h & e & l \\ f & -f & 0 & -m & k & A \end{bmatrix}; \qquad (4P:11)$$

if the y axis is taken normal to one of the edges of the rhombohedron, the tensor (4P:10) is changed to

$$\begin{bmatrix} a & b & c & -k & -m & -f \\ b & a & c & k & m & f \\ d & d & T_{33} & 0 & 0 & 0 \\ -l & l & 0 & e & -h & n \\ -n & n & 0 & h & e & -l \\ f & -f & 0 & m & -k & A \end{bmatrix}. \qquad (4P:12)$$

In the kind $r3mR$, the tensor in one state is

$$\begin{bmatrix} a & b & c & k & 0 & 0 \\ b & a & c & -k & 0 & 0 \\ d & d & T_{33} & 0 & 0 & 0 \\ l & -l & 0 & e & 0 & 0 \\ 0 & 0 & 0 & 0 & e & l \\ 0 & 0 & 0 & 0 & k & A \end{bmatrix} \qquad (4P:13)$$

or

$$\begin{bmatrix} a & b & c & 0 & -m & 0 \\ b & a & c & 0 & m & 0 \\ d & d & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & e & 0 & n \\ -n & n & 0 & 0 & e & 0 \\ 0 & 0 & 0 & m & 0 & A \end{bmatrix}, \qquad (4P:14)$$

where $A=\frac{1}{2}(a-b)$, according as to which axis, x or y, is taken normal to one of the mirror planes of symmetry. By S.T. the tensor (4P:13) or (4P:14) is unchanged.

In the kinds $r3P$'s, the tensor in one state is (4P:10). By S.T. this is unchanged for $r3P$-I and changed for $r3P$-II to

$$\begin{bmatrix} a & b & c & -k & m & f \\ b & a & c & k & -m & -f \\ d & d & T_{33} & 0 & 0 & 0 \\ -l & l & 0 & e & h & -n \\ n & -n & 0 & -h & e & -l \\ -f & f & 0 & -m & -k & A \end{bmatrix}. \qquad (4P:15)$$

If the x axis is taken normal to one of the side faces of the unit-cell hexagonal prism, then by S.T. the tensor (4P:10) is changed for $r3P$-III to (4P:11) and for $r3P$-IV to (4P:12); if the y axis is taken normal to one of the side faces of the hexagonal prism, the tensor (4P:10) is changed for $r3P$-III to (4P:12) and for $r3P$-IV to (4P:11).

In the kinds $r3mP$-I and $r3mP$-II, if the x axis is taken normal to one of the mirror planes of symmetry, the tensor in one state is (4P:13). By S.T. this is unchanged for $r3mP$-I and changed for $r3mP$-II to

$$\begin{bmatrix} a & b & c & -k & 0 & 0 \\ b & a & c & k & 0 & 0 \\ d & d & T_{33} & 0 & 0 & 0 \\ -l & l & 0 & e & 0 & 0 \\ 0 & 0 & 0 & 0 & e & -l \\ 0 & 0 & 0 & 0 & -k & A \end{bmatrix}. \qquad (4P:16)$$

If the y axis is taken normal to one of the mirror planes of symmetry, the tensor in one state is (4P:14). By S.T. this is unchanged for $r3mP$-I and changed for $r3mP$-II to

$$\begin{bmatrix} a & b & c & 0 & m & 0 \\ b & a & c & 0 & -m & 0 \\ d & d & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & e & 0 & -n \\ n & -n & 0 & 0 & e & 0 \\ 0 & 0 & 0 & -m & 0 & A \end{bmatrix}. \qquad (4P:17)$$

3.7. Axial Tensor of Rank Four

In the kind $r1$, the tensor in one state comprises 36 independent elements. This tensor is reversed in sign by S.T. In the kind rm, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & T_{14} & T_{15} & 0 \\ 0 & 0 & 0 & T_{24} & T_{25} & 0 \\ 0 & 0 & 0 & T_{34} & T_{35} & 0 \\ T_{41} & T_{42} & T_{43} & 0 & 0 & T_{46} \\ T_{51} & T_{52} & T_{53} & 0 & 0 & T_{56} \\ 0 & 0 & 0 & T_{64} & T_{65} & 0 \end{bmatrix} \qquad (4A:1)$$

in the first setting and

$$\begin{bmatrix} 0 & 0 & 0 & T_{14} & 0 & T_{16} \\ 0 & 0 & 0 & T_{24} & 0 & T_{26} \\ 0 & 0 & 0 & T_{34} & 0 & T_{36} \\ T_{41} & T_{42} & T_{43} & 0 & T_{45} & 0 \\ 0 & 0 & 0 & T_{54} & 0 & T_{56} \\ T_{61} & T_{62} & T_{63} & 0 & T_{65} & 0 \end{bmatrix} \qquad (4A:2)$$

in the second setting. This tensor is reversed in sign by S.T.

In the kind $r2$, the tensor in one state is

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} & 0 & 0 & T_{16} \\ T_{21} & T_{22} & T_{23} & 0 & 0 & T_{26} \\ T_{31} & T_{32} & T_{33} & 0 & 0 & T_{36} \\ 0 & 0 & 0 & T_{44} & T_{45} & 0 \\ 0 & 0 & 0 & T_{54} & T_{55} & 0 \\ T_{61} & T_{62} & T_{63} & 0 & 0 & T_{66} \end{bmatrix} \qquad (4A:3)$$

in the first setting and

$$\begin{bmatrix} T_{11} & T_{12} & T_{13} & 0 & T_{15} & 0 \\ T_{21} & T_{22} & T_{23} & 0 & T_{25} & 0 \\ T_{31} & T_{32} & T_{33} & 0 & T_{35} & 0 \\ 0 & 0 & 0 & T_{44} & 0 & T_{46} \\ T_{51} & T_{52} & T_{53} & 0 & T_{55} & 0 \\ 0 & 0 & 0 & T_{64} & 0 & T_{66} \end{bmatrix} \qquad (4A:4)$$

in the second setting. This tensor is reversed in sign by S.T.

In the kind *rmm*2, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & T_{16} \\ 0 & 0 & 0 & 0 & 0 & T_{26} \\ 0 & 0 & 0 & 0 & 0 & T_{36} \\ 0 & 0 & 0 & 0 & T_{45} & 0 \\ 0 & 0 & 0 & T_{54} & 0 & 0 \\ T_{61} & T_{62} & T_{63} & 0 & 0 & 0 \end{bmatrix}. \quad (4A{:}5)$$

This is reversed in sign by S.T.

In the kinds *r*4-I and *r*4-II, the tensor in one state is

$$\begin{bmatrix} h & k & l & 0 & 0 & b \\ k & h & l & 0 & 0 & -b \\ m & m & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & n & a & 0 \\ 0 & 0 & 0 & -a & n & 0 \\ c & -c & 0 & 0 & 0 & T_{66} \end{bmatrix}. \quad (4A{:}6)$$

For *r*4-I, this is changed by S.T. to the tensor of opposite sign, i.e.,

$$\begin{bmatrix} -h & -k & -l & 0 & 0 & -b \\ -k & -h & -l & 0 & 0 & b \\ -m & -m & -T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & -n & -a & 0 \\ 0 & 0 & 0 & a & -n & 0 \\ -c & c & 0 & 0 & 0 & -T_{66} \end{bmatrix}. \quad (4A{:}7)$$

For *r*4-II, if the x axis is taken normal or at 45° to one of the side faces of the unit-cell tetragonal prism, the tensor (4A:6) is changed by S. T. to

$$\begin{bmatrix} h & k & l & 0 & 0 & -b \\ k & h & l & 0 & 0 & b \\ m & m & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & n & -a & 0 \\ 0 & 0 & 0 & a & n & 0 \\ -c & c & 0 & 0 & 0 & T_{66} \end{bmatrix}. \quad (4A{:}8)$$

In the kind *r*4*mm*, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & b \\ 0 & 0 & 0 & 0 & 0 & -b \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a & 0 \\ 0 & 0 & 0 & -a & 0 & 0 \\ c & -c & 0 & 0 & 0 & 0 \end{bmatrix}. \quad (4A{:}9)$$

This is reversed in sign by S.T.

In the kinds *r*6-I and *r*6-II, the tensor in one state is

$$\begin{bmatrix} h & k & l & 0 & 0 & b \\ k & h & l & 0 & 0 & -b \\ m & m & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & n & a & 0 \\ 0 & 0 & 0 & -a & n & 0 \\ -b & b & 0 & 0 & 0 & A \end{bmatrix}, \quad (4A{:}10)$$

where $A=\frac{1}{2}(h-k)$. (The direction of the x axis is free.) By S.T. this is changed for *r*6-I to the tensor of opposite sign, i.e.,

$$\begin{bmatrix} -h & -k & -l & 0 & 0 & -b \\ -k & -h & -l & 0 & 0 & b \\ -m & -m & -T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & -n & -a & 0 \\ 0 & 0 & 0 & a & -n & 0 \\ b & -b & 0 & 0 & 0 & -A \end{bmatrix}, \quad (4A{:}11)$$

and for *r*6-II to

$$\begin{bmatrix} h & k & l & 0 & 0 & -b \\ k & h & l & 0 & 0 & b \\ m & m & T_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & n & -a & 0 \\ 0 & 0 & 0 & a & n & 0 \\ b & -b & 0 & 0 & 0 & A \end{bmatrix}. \quad (4A{:}12)$$

In the kind *r*6*mm*, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & b \\ 0 & 0 & 0 & 0 & 0 & -b \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a & 0 \\ 0 & 0 & 0 & -a & 0 & 0 \\ -b & b & 0 & 0 & 0 & 0 \end{bmatrix}. \quad (4A{:}13)$$

(The direction of the x axis is free.) This is reversed in sign by S.T.

In the kinds *r*3*R*-I and *r*3*R*-II, the tensor in one state is

$$\begin{bmatrix} h & k & l & f & -d & b \\ k & h & l & -f & d & -b \\ m & m & T_{33} & 0 & 0 & 0 \\ g & -g & 0 & n & a & e \\ -e & e & 0 & -a & n & g \\ -b & b & 0 & d & f & A \end{bmatrix}, \quad (4A{:}14)$$

where $A=\frac{1}{2}(h-k)$. For *r*3*R*-I, this is changed by S.T. to the tensor of opposite sign, i.e.,

$$\begin{bmatrix} -h & -k & -l & -f & d & -b \\ -k & -h & -l & f & -d & b \\ -m & -m & -T_{33} & 0 & 0 & 0 \\ -g & g & 0 & -n & -a & -e \\ e & -e & 0 & a & -n & -g \\ b & -b & 0 & -d & -f & -A \end{bmatrix}. \quad (4A{:}15)$$

For *r*3*R*-II, if the x axis is taken normal to one of the edges of the unit-cell rhombohedron, the tensor (4A:14) is changed by S.T. to

$$\begin{bmatrix} h & k & l & f & d & -b \\ k & h & l & -f & -d & b \\ m & m & T_{33} & 0 & 0 & 0 \\ g & -g & 0 & n & -a & -e \\ e & -e & 0 & a & n & g \\ b & -b & 0 & -d & f & A \end{bmatrix}; \quad (4A\text{-}16)$$

if the y axis is taken normal to one of the edges of the rhombohedron, the tensor (4A:14) is changed to

$$\begin{bmatrix} h & k & l & -f & -d & -b \\ k & h & l & f & d & b \\ m & m & T_{33} & 0 & 0 & 0 \\ -g & g & 0 & n & -a & e \\ -e & e & 0 & a & n & -g \\ b & -b & 0 & d & -f & A \end{bmatrix}. \quad (4A:17)$$

In the kind $r3mR$, the tensor in one state is

$$\begin{bmatrix} 0 & 0 & 0 & 0 & -d & b \\ 0 & 0 & 0 & 0 & d & -b \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a & e \\ -e & e & 0 & -a & 0 & 0 \\ -b & b & 0 & d & 0 & 0 \end{bmatrix} \quad (4A:18)$$

or

$$\begin{bmatrix} 0 & 0 & 0 & f & 0 & b \\ 0 & 0 & 0 & -f & 0 & -b \\ 0 & 0 & 0 & 0 & 0 & 0 \\ g & -g & 0 & 0 & a & 0 \\ 0 & 0 & 0 & -a & 0 & g \\ -b & b & 0 & 0 & f & 0 \end{bmatrix} \quad (4A:19)$$

according as to which axis, x or y, is taken normal to one of the mirror planes of symmetry. By S.T. the tensor (4A:18) or (4A:19) is reversed in sign.

In the kinds $r3P$'s, the tensor in one state is (4A:14). By S.T. this is changed for $r3P$-I to (4A:15) and for $r3P$-II to

$$\begin{bmatrix} -h & -k & -l & f & -d & -b \\ -k & -h & -l & -f & d & b \\ -m & -m & -T_{33} & 0 & 0 & 0 \\ g & -g & 0 & -n & -a & e \\ -e & e & 0 & a & -n & g \\ b & -b & 0 & d & f & -A \end{bmatrix}. \quad (4A:20)$$

If the x axis is taken normal to one of the side faces of the unit-cell hexagonal prism, then by S.T. the tensor (4A:14) is changed for $r3P$-III to (4A:16) and for $r3P$-IV to (4A:17); if the y axis is taken normal to one of the side faces of the hexagonal prism, the tensor (4A:14) is changed for $r3P$-III to (4A:17) and for $r3P$-IV to (4A:16).

In the kinds $r3mP$-I and $r3mP$-II, if the x axis is taken normal to one of the mirror planes of symmetry, the tensor in one state is (4A:18). By S.T. this is changed for $r3mP$-I to the tensor of opposite sign, i.e.,

$$\begin{bmatrix} 0 & 0 & 0 & 0 & d & -b \\ 0 & 0 & 0 & 0 & -d & b \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -a & -e \\ e & -e & 0 & a & 0 & 0 \\ b & -b & 0 & -d & 0 & 0 \end{bmatrix} \quad (4A:21)$$

and for $r3mP$-II to

$$\begin{bmatrix} 0 & 0 & 0 & 0 & -d & -b \\ 0 & 0 & 0 & 0 & d & b \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -a & e \\ -e & e & 0 & a & 0 & 0 \\ b & -b & 0 & d & 0 & 0 \end{bmatrix}. \quad (4A:22)$$

If the y axis is taken normal to one of the mirror planes of symmetry, the tensor in one state is (4A:19). By S.T. this is changed for $r3mP$-I to the tensor of opposite sign, i.e.,

$$\begin{bmatrix} 0 & 0 & 0 & -f & 0 & -b \\ 0 & 0 & 0 & f & 0 & b \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -g & g & 0 & 0 & -a & 0 \\ 0 & 0 & 0 & a & 0 & -g \\ b & -b & 0 & 0 & -f & 0 \end{bmatrix} \quad (4A:23)$$

and for $r3mP$-II to

$$\begin{bmatrix} 0 & 0 & 0 & f & 0 & -b \\ 0 & 0 & 0 & -f & 0 & b \\ 0 & 0 & 0 & 0 & 0 & 0 \\ g & -g & 0 & 0 & -a & 0 \\ 0 & 0 & 0 & a & 0 & g \\ b & -b & 0 & 0 & f & 0 \end{bmatrix}. \quad (4A:24)$$

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