Group-theoretical definition of crystal-structure types

Bulletin of the College of Science
University of the Ryukyus No.41:31-48 (1986)

Group-theoretical definition of crystal-structure types

Masahiko HOSOYA

Department of Physics, College of Science,
University of the Ryukyus,
Nishihara, Okinawa, 903-01 JAPAN

(Received 29 October, 1985)

Abstract

A mathematically unambiguous definition is given to crystal-structure types for the first time. This enables us to enumerate all the possible crystal-structure types systematically. The classification system is also presented which consists of species, genuses, and families. A species is a refined concept of crystal-structure type, while a genus is a set of crystals whose chemical formulae for primitive cells are similar to each other. The numbers of species in genus A, AB, and A_2 are shown to be 14, 51, and 29 respectively. Atomic arrangements of these structures are given in tables and figures.

I. Introduction

The concept of a crystal-structure type has long been known as a convenient tool to specify the atomic allocation of a crystal. It was introduced empirically so that its rigorous definition has not been given. On the other hand, the rigorous enumeration of crystal-structure types has been started by several authors since about 10 years ago (Niggli, 1971; Sakamoto, 1974; Hosoya, 1980; Hosoya, 1982a; Hosoya, 1982b; Hosoya, 1983; Sakamoto, Kida, Hiraga & Murata, 1983). Their results coincide with each other essentially. Hence it seems to be true that crystal-structure types are unambiguous mathematical objects such as 14 Bravais lattices, 32 point groups or 230 space groups. The present paper intends to define a crystal-structure type mathematically by extending the concept of symmetry operations in crystallography.

The essence of the present paper lies in that every crystal-structure type is defined by a corresponding group. The group specifies the crystal as finely as possible with respect to symmetry. This may contradict the usual belief that a space group is the most detailed group-theoretical concept in crystallography. As far as we concern the transformation of the coordinate system or the whole space, there can not be more detailed one, for a space group gives the complete knowledge of the symmetry elements in the given crystal. However a space group does not concern the transformation of individual atoms explicitly. Thus if we pay attention to the allocation of atoms, we have a chance to meet another group which gives more information

than a space group. Such consideration leads us to the idea that there can be a more detailed rank than space group.

All the space group operations transfer atoms to the positions formerly occupied by other atoms of the same kind. Hence the operations can be regarded as the permutation of the atoms and the space group is translated into a permutation group. This new viewpoint produces all the results obtained in the present paper. We make every crystal-structure type correspond to a permutation group which is realizable as a space group. Hereafter these realizable permutation group will be called a **structure group**. Very often a space group corresponds to more than one structure groups even if the compositions of the crystal are the same. Hence the structure groups give us more detailed classification of the crystal-structure types than the space groups. Another merit of defining a crystal-structure type by its corresponding permutation group is its simplicity of distinction between any two crystal-structure types. Whether any two crystals are equivalent or not as a crystal-structure type is determined by whether their permutation groups are group-theoretically equivalent or not. Further details are given in the next section.

Our next problem is how to get a simple representation matrix for a structure group. Since there are an infinite number of atoms in a crystal, a straightforward treatment of permutation is impossible. We must choose a representative set of parameters which can determine the whole crystal. Obviously one primitive cell is sufficient enough to specify the crystal. We adopt the three edge vectors of the primitive cell, a, b, c, and the position vectors of the atoms in the cell, $x_1, x_2, \ldots, x_n$, where n is the number of atoms per cell. Thus our problem is reduced to finding an appropriate representation to transform $(a, b, c, x_1, x_2, \ldots, x_n)$.

We are familiar with the following expression which directly shows that a space group operation is an affine transformation

$$x' = R \cdot x + t. \qquad (1)$$

However this is quite inadequate to describe the interchange of atoms, for the parameter matrices R and t are the same for any atoms. We must look for another representation by any means. There can be various versions which include the one proposed in the previous papers (Hosoya, 1979; Hosoya, 1980), but the simplest one is the following.

$$x' = x + T. \qquad (2)$$

The parameter matrix T differs from one atom to another according to their positions. The concrete representation is given in the next section.

Once every crystal-structure type is related to the corresponding structure group, the enumeration and classification can be performed in a mathematically unambiguous way. All the possible structures, the number of which is of course infinite, construct a magnificent classification system which reminds us of biology. To each rank of this system, we will apply the same nomenclature as that of biology. Thus the lowest rank of classification is called a **species**, and it ascends to a **genus** and a **family** successively. The higher ranks than family are not needed in the present classification. It should be noted that the meaning of each rank is completely different from Sakamoto's one where the nomenclature is also borrowed from biology (Sakamoto, 1974; Sakamoto, Kida, Hiraga & Murata, 1983).

Since a species is the most fundamental concept, its geometrical meaning should be mentioned briefly here. A species provides the complete information about the permutations of atoms caused by the space group operations. The most detailed information is whether each atom is interchanged or kept invariant under an operation. The question is reduced to whether each atom lies on a plane of symmetry, a line of symmetry, or a point of symmetry specified by the operation (Bradley & Cracknell, 1972). Thus if any two crystal-structure types belong to the same species, their allocation of atoms on each plane, line or point of symmetry are identical. We may say that the idea of a species is only the refined one which has been vaguely called a crystal-structure type or merely a crystal structure. For instance many wellknown structures such as f.c.c., b.c.c., diamond, NaCl, CsCl or perovskite one are regarded as species.

In order to classify a set of groups, we should always follow Aizu's method which derives all the groups as a subgroup of the **prototypic group** (Aizu, 1962; Aizu, 1966; Aizu, 1969; Aizu, 1970; Aizu, 1979). In the present case, the prototypic group is easily obtained by collecting all the relevant operations and their products if the composition in the primitive cell is given. Though the prototypic group is an infinite group, the derivation of the subgroups can be performed similarly. The group-subgroup relations construct the hierarchy of species. Thus we have a genealogical tree of species which supplies the base of our classification system.

II. Species and Genus of Crystal-Structure Types

In order to describe a crystal structure, its composition of a primitive cell must be known. Thus we regard the composition as an important category of our classification and call it a genus. The name of a genus is naturally given by the chemical formula of its composition. However ordinary chemical formulae are inadequate. Since our crystallographic study does not concern the nature of each chemical element itself nor chemical bond between them, the atomic symbols and their seating order have no meaning in the formula. We only need to know whether any two atoms belong to the same chemical element or not. Hence in the chemical formula we arrange the atomic symbols in increasing order of their suffices and substitute the alphabet from A to Z for the atomic symbols one by one.

Once a genus is given, possible structures can be classified into a finite number of species. The classification should be done according to their structure groups, that is, the permutation groups which are realizable as space groups. Since a primitive cell determines the whole crystal completely, the independent variables are the three primitive translation vectors a, b, c and the position vectors of the atoms in the cell, $x_1, x_2, \ldots, x_n$. The other primitive cells are assumed to transform uniquely as if they were linkaged to the first one. That is, if we transform a, b, c, $x_1, x_2, \ldots, x_n$ into $a', b', c', x_1', x_2', \ldots, x_n'$, then any atom at a position $p=n_1 \cdot a+n_2 \cdot b+n_3 \cdot c+x_i$ is transformed into $p'=n_1 \cdot a'+n_2 \cdot b'+n_3 \cdot c'+x_i'$. Now the set of vectors $(a,b,c,x_1, \ldots, x_n)$ will be called a basis of primitive cell (**bpc**). As is stated in section I, the structure group is represented by the translation of atoms in Eq. (2).

$$x'=T+x \qquad (2)$$

If we use the vectors a, b, c as the bases of T, Eq. (2) can be written as follows.

$$x' = (T_1, T_2, T_3, 1) \begin{bmatrix} a \\ b \\ c \\ x \end{bmatrix} \tag{3}$$

We can also consider that a, b, and c themselves are transformed in the similar way, but these reduce to the usual linear transformation as follows.

$$\begin{bmatrix} a' \\ b' \\ c' \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} \tag{4}$$

It should be noted that a', b', and c' are the edge vectors of the transformed primitive cell and not a position vector whose origin is fixed. (See Figure 1.) Thus the transformation of the whole bpc is represented as follows.

$$\begin{bmatrix} a' \\ b' \\ c' \\ x_1' \\ \vdots \\ x_n' \end{bmatrix} = \left[\begin{array}{ccc:c:ccc} A_{11} & A_{12} & A_{13} & 0 & \multicolumn{3}{c}{\multirow{3}{*}{0}} \\ A_{21} & A_{22} & A_{23} & 0 & & & \\ A_{31} & A_{32} & A_{33} & 0 & & & \\ \hdashline T_{11} & T_{12} & T_{13} & 1 & 0 & \cdots & 0 \\ & & & \vdots & & & \\ T_{n1} & T_{n2} & T_{n3} & 0 & \cdots & 0 & 1 \end{array}\right] \begin{bmatrix} a \\ b \\ c \\ x_1 \\ \vdots \\ x_n \end{bmatrix} \tag{5}$$

The components of the transformation matrix should be restricted so that it can be realized as an actual space group operation.

The matrix (A_{ij}) should be unimodular, i.e., the value of its determinant must be +1, because the volume of the primitive cell must be held constant.

Next we must consider the condition that the bpc is transformed into another bpc of the same crystal. Since we have assumed that the vectors a, b, c are the primitive translation vectors, any translation vectors are the sums of integer multiples of a, b, c. This means that the components (A_{ij}) must be integers for a', b', c' to be also the primitive translation vectors. (Such integral unimodular matrices A_{ij} coincide with those used in defining Bravais arithmetic crystal class Z which was introduced by Neubüser, Wondratschek and Bülow (1971).) Similarly integral components of (T_{ij}) guarantees that every atom is transformed to the equivalent position by translational symmetry. However the identical atoms may exist in the same primitive cell, and the transformation may be the interchange between such atoms. Hence in compensation for the requirement that T_{ij} should be an integer, the identify matrix of the lower right part should be replaced to a permutation matrix which has only one unity component for each row and column, and zeros for the others.

Thus by all the above conditions we have the following transformation.

$$\begin{pmatrix} a' \\ b' \\ c' \\ x_1' \\ \vdots \\ x_n' \end{pmatrix} = \left[\begin{array}{c|c} \text{integral} & 0 \\ \text{unimodular} & 0 \\ & 0 \\ \hline \text{integral} & \text{permutation} \end{array}\right] \begin{pmatrix} a \\ b \\ c \\ x_1 \\ \vdots \\ x_n \end{pmatrix} \tag{6}$$

Now the prototypic group of a genus is constructed of all the possible operations of the above type. An example of the transformation in Eq. (6) is shown in Figure 1. Obviously they do not always coincide with the ordinary symmetry operations such as rotations or reflections.

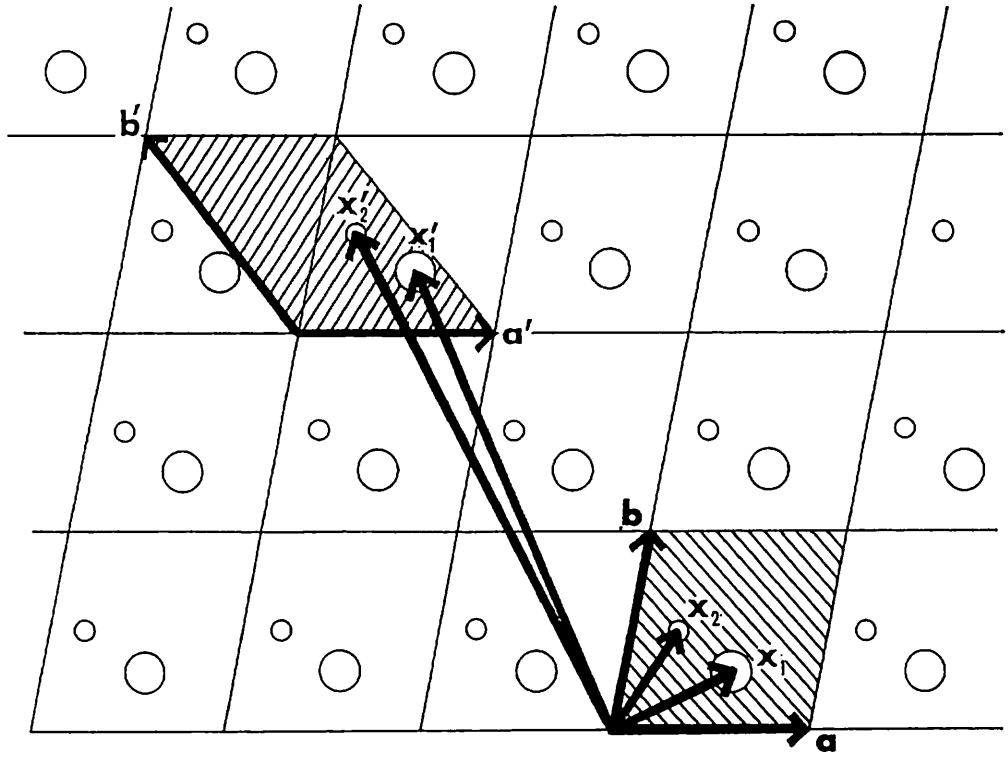

Figure 1. A two-dimensional example of transformation used in the present paper to define a crystal-structure type. All the atoms are overlapped on the other ones by an affine transformation which does not always coincide with ordinary symmetry operations such as rotations or reflections. The transformation of vectors a, b, x_1, x_2 into a', b', x_1', x_2' is represented as follows.

$$\begin{pmatrix} a' \\ b' \\ x_1' \\ x_2' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ -2 & 2 & 1 & 0 \\ -2 & 2 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ x_1 \\ x_2 \end{pmatrix}$$

However if some appropriate relations hold between the components of bpc (such as $a=b=c$, or $x_1 \cdot a=0$, etc.), some operations may coincide with the ordinary symmetry operations. That is, the transformation (6) for such an operation can be also written as follows:

$$\begin{aligned} a' &= R\cdot a, \\ b' &= R\cdot b, \\ c' &= R\cdot c, \\ x_1' &= R\cdot x_1 + t, \\ &\vdots \\ x_n' &= R\cdot x_n + t, \end{aligned} \tag{7}$$

where R and t are some rotational matrix and some translational vector respectively. (It should be noted that the transformation of a, b, and c has no translational part even when the corresponding space group is non-symmorphic.) Such operations form a subgroup of the prototypic group which is a representation of the corresponding space group. A species is identified by assigning such a subgroup to the bpc and the subgroup is called its structure group. If more than one subgroup is applicable to the same bpc, then the largest subgroup is assigned.

As is well known in group theory, a subgroup $(\mathbf{Y}_1, \mathbf{Y}_2, \ldots)$ of a group G is equivalent to the subgroup $(\mathbf{XY}_1\mathbf{X}^{-1}, \mathbf{XY}_2\ \mathbf{X}^{-1}, \ldots)$ where X is an arbitrary element of G. Thus two subgroups correspond to the same species, if and only if they are inner automorphic to each other. It is this criterion of equivalence that makes the concept of a species unambiguous. So far such a statement has never been given explicitly. Most of the operations X used in the similarity transformations are of course not realizable as the ordinary symmetry operation for the given bpc $(a, b, c, x_1, x_2, \ldots)$. Fail to notice such operations as a symmetry element may have delayed the establishment of the mathematical concept of crystal-structure types.

Moreover a similar equivalence arises from the arbitrariness of our definition of a genus. The chemical formula of a genus is a representative of all the versions which are obtained by the interchange of atomic symbols betweeen the elements which have the same suffices. For instance, genus $\mathbf{AB_2C_2}$ means either of two variations which might be written symbolically as $\mathbf{AB_2C_2}$ and $\mathbf{AC_2B_2}$. Thus such interchange between atoms of different kind should be included in the operations X of the above similarity transformation.

The name of a species is given by the following three symbols separated by ":".

(1) The degree of freedom allowed in the crystal of the species. (The number of parameters that can be changed without any change of symmetry.)

(2) International symbol of space group assigned to the species.

(3) A sequence of Wyckoff notations which specify each atomic position in the order of the formula of genus. If more than one expression is possible, the most preceding one in the alphabetical order is adopted.

III. An Example: Genus AB

A simple example of determining the species is given in the following. The simplest genus is A, but its species coincide with the wellknown 14 Bravais lattice types. Then we classify

the next simplest genus AB. Crystals of genus AB are given by bpc (a, b, c, x_1, x_2). The transformations are represented as a 5×5 matrix and a set of all of them makes up the prototypic group of the genus. Among them the generating elements are as follows. (The name of each matrix is chosen so that it should suggest the corresponding rotation or reflection when it is realized as a space-group operation for an appropriate bpc.)

$$S_6 = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -1 & -1 & -1 & 0 & 1 \end{pmatrix}, \quad C_4 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -1 & 1 & -1 & 0 & 1 \end{pmatrix},$$

$$m = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad C_4' = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 1 \end{pmatrix},$$

$$S_4 = \begin{pmatrix} -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad m' = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 1 \end{pmatrix},$$

$$C_6 = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad C_3 = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 1 \end{pmatrix},$$

$$C_4'' = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{8}$$

In addition to these, there are of course the following three primitive translations and their inverses.

$$T_a = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{pmatrix} \quad T_b = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{pmatrix} \quad T_c = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{pmatrix}$$

These operations produce 51 species in genus AB as is shown in Table 1. The crystal structures of 51 species are shown in Figure 2 where each conventional unit cell is drawn. The hierarchy of the species of genus AB is given in Figure 3, where if two species are connected to

Table 1. Species in genus AB.

Species	Generating elements	The position of atom B in the conventional unit cell with the atom A at the origin
1 : $Fm\bar{3}m$: ab (NaCl)	S_6, C_4, m	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
1 : $Pm\bar{3}m$: ab (CsCl)	S_6, C_4', m	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
1 : $F\bar{4}3m$: ac (Zinc blende)	$(S_6)^2$, S_4, m	$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$
2 : P6/mmm : ab	C_6, m, $(C_4')^2 \cdot (S_6)^3$	$(0, 0, \frac{1}{2})$
2 : $P\bar{6}m2$: ac	C_3, m, m′	$(\frac{1}{3}, \frac{2}{3}, 0)$
2 : $P\bar{6}m2$: ad (WC)	C_3, m, $(C_4')^2 \cdot (S_6)^3$	$(\frac{1}{3}, \frac{2}{3}, \frac{1}{2})$
2 : $R\bar{3}m$: ab (CuPt)	S_6, m	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
2 : I4/mmm : ab	C_4, m, $(C_4)^2 \cdot (S_6)^3$	$(0, 0, \frac{1}{2})$
2 : P4/mmm : ab	C_4'', m, $(C_4')^2 \cdot (S_6)^3$	$(0, 0, \frac{1}{2})$
2 : P4/mmm : ac	C_4', m, m′	$(\frac{1}{2}, \frac{1}{2}, 0)$
2 : P4/mmm : ad	C_4', m, $(C_4')^2 \cdot (S_6)^3$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
2 : $I\bar{4}m2$: ac	S_4, m	$(0, \frac{1}{2}, \frac{1}{4})$
3 : P6mm : aa	C_6, m	$(0, 0, z)$
3 : R3m : aa	$(S_6)^2$, m	(x, x, x)
3 : P3m1 : ab	C_3, m	$(\frac{1}{3}, \frac{2}{3}, z)$
3 : I4mm : aa	C_4, m	$(0, 0, z)$
3 : P4mm : aa	C_4'', m	$(0, 0, z)$
3 : P4mm : ab	C_4', m	$(\frac{1}{2}, \frac{1}{2}, z)$
3 : Immm : ab	$(C_4)^2$, m, $(C_4)^2 \cdot (S_6)^3$	$(0, \frac{1}{2}, \frac{1}{2})$
3 : Fmmm : ab	$(C_4)^2$, $C_4 \cdot$ m, $(C_4)^2 \cdot (S_6)^3$	$(0, 0, \frac{1}{2})$
3 : Cmmm : ab	$(C_4')^2$, m, m′	$(\frac{1}{2}\ 0\ 0)$
3 : Cmmm : ac	$(C_4')^2$, m, $(C_4')^2 \cdot (S_6)^3$	$(\frac{1}{2}, 0, \frac{1}{2})$
3 : Cmmm : ad	$(C_4'')^2$, m, $(C_4')^2 \cdot (S_6)^3$	$(0, 0, \frac{1}{2})$
3 : Pmmm : ab	$(C_4')^2$, $C_4' \cdot$ m, $(C_4')^2 \cdot (S_6)^3$	$(\frac{1}{2}, 0, 0)$
3 : Pmmm : ad	$(C_4')^2$, $C_4' \cdot$ m, m′	$(\frac{1}{2}, 0, \frac{1}{2})$
3 : Pmmm : ah	$(C_4'')^2$, $C_4'' \cdot$ m, $(C_4')^2 \cdot (S_6)^3$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
3 : F222 : ac	$(S_4)^2$, $S_4 \cdot$ m	$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$

Table 1. Species in genus AB. (Continued)

Species	Generating elements	The position of atom B in the conventional unit cell with the atom A at the origin
4 : Imm2 : aa	$(C_4)^2$, m	$(0, 0, z)$
4 : Imm2 : ab	$(S_4)^2$, m	$(0, \frac{1}{2}, z)$
4 : Fmm2 : aa	$(C_4)^2$, $C_4 \cdot$ m	$(0, 0, z)$
4 : Amm2 : aa	m, m′	$(0, 0, z)$
4 : Amm2 : ab	m, $(C_4')^2 \cdot (S_6)^3$	$(\frac{1}{2}, 0, z)$
4 : Cmm2 : aa	m, $(C_4'')^2$	$(0, 0, z)$
4 : Cmm2 : ab	m, $(C_4')^2$	$(0, \frac{1}{2}, z)$
4 : Pmm2 : aa	$(C_4'')^2$, $C_4'' \cdot$ m	$(0, 0, z)$
4 : Pmm2 : ab	$(C_4')^2 \cdot (S_6)^3$, $C_4'' \cdot$ m	$(0, \frac{1}{2}, z)$
4 : Pmm2 : ad	$(C_4')^2$, $C_4' \cdot$ m	$(\frac{1}{2}, \frac{1}{2}, z)$
4 : B2/m : ab	m, $m \cdot (S_6)^3$	$(0, 0, \frac{1}{2})$
4 : B2/m : ac	$(C_4)^2$, $(C_4)^2 \cdot (S_6)^3$	$(0, \frac{1}{2}, 0)$
4 : P2/m : ab	$(C_4'')^2$, $(C_4')^2 \cdot (S_6)^3$	$(0, 0, \frac{1}{2})$
4 : P2/m : ac	$(C_4')^2$, m′	$(0, \frac{1}{2}, 0)$
4 : P2/m : ae	$(C_4')^2$, $(C_4')^2 \cdot (S_6)^3$	$(\frac{1}{2}, 0, \frac{1}{2})$
5 : B2 : aa	$(C_4)^2$	$(0, 0, z)$
5 : B2 : ab	$(S_4)^2$	$(0, \frac{1}{2}, z)$
5 : P2 : aa	$(C_4'')^2$	$(0, 0, z)$
5 : P2 : ab	$(C_4')^2$	$(0, \frac{1}{2}, z)$
6 : Bm : aa	m	$(x, y, 0)$
6 : Pm : aa	m′	$(x, y, 0)$
6 : Pm : ab	$(C_4')^2 \cdot (S_6)^3$	$(x, y, \frac{1}{2})$
6 : $P\bar{1}$: ab	$(S_6)^3$	$(0, 0, \frac{1}{2})$
9 : P1 : aa	E (Identity element)	(x, y, z)

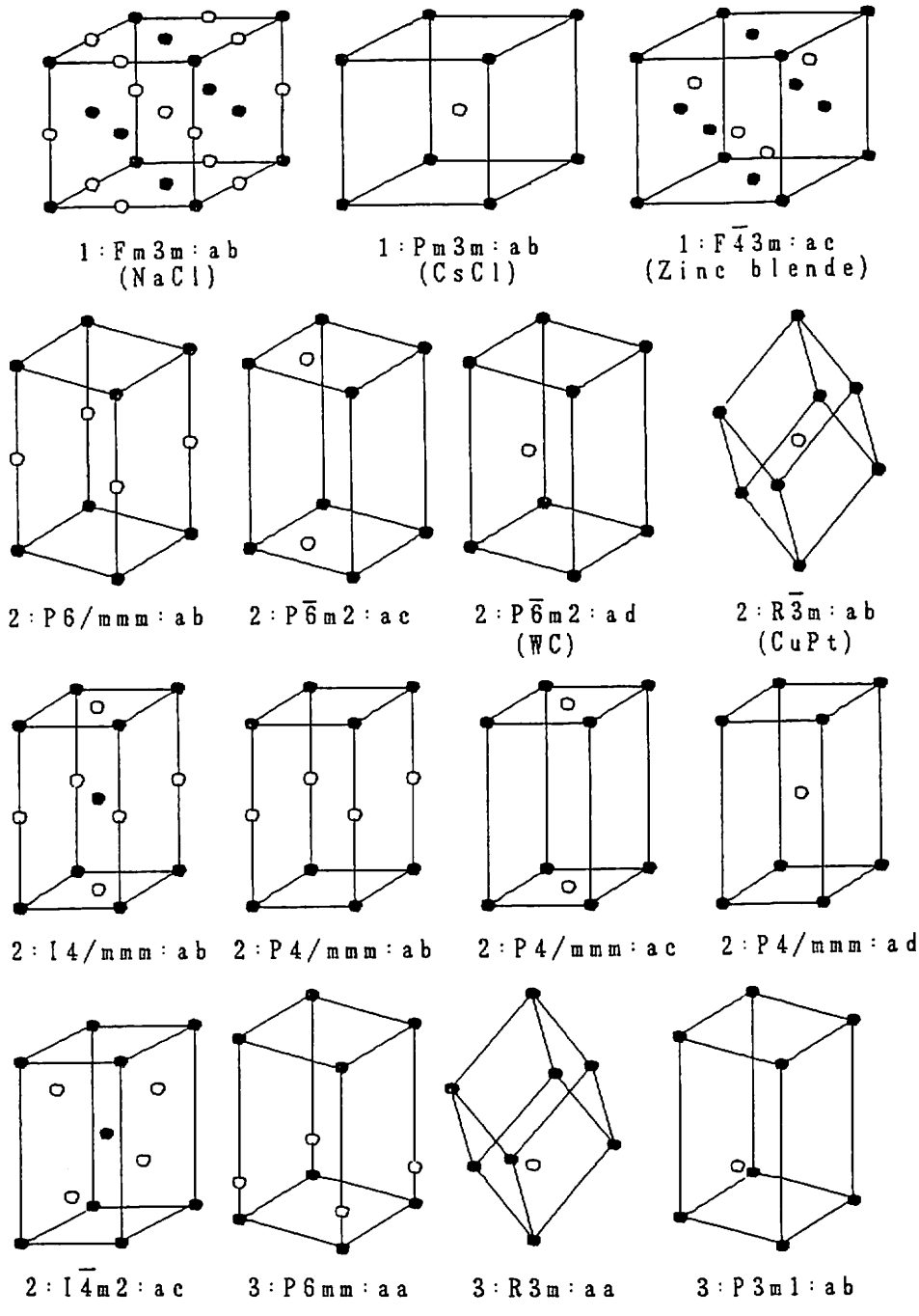

Figure 2. Atomic arrangement of species in genus AB.

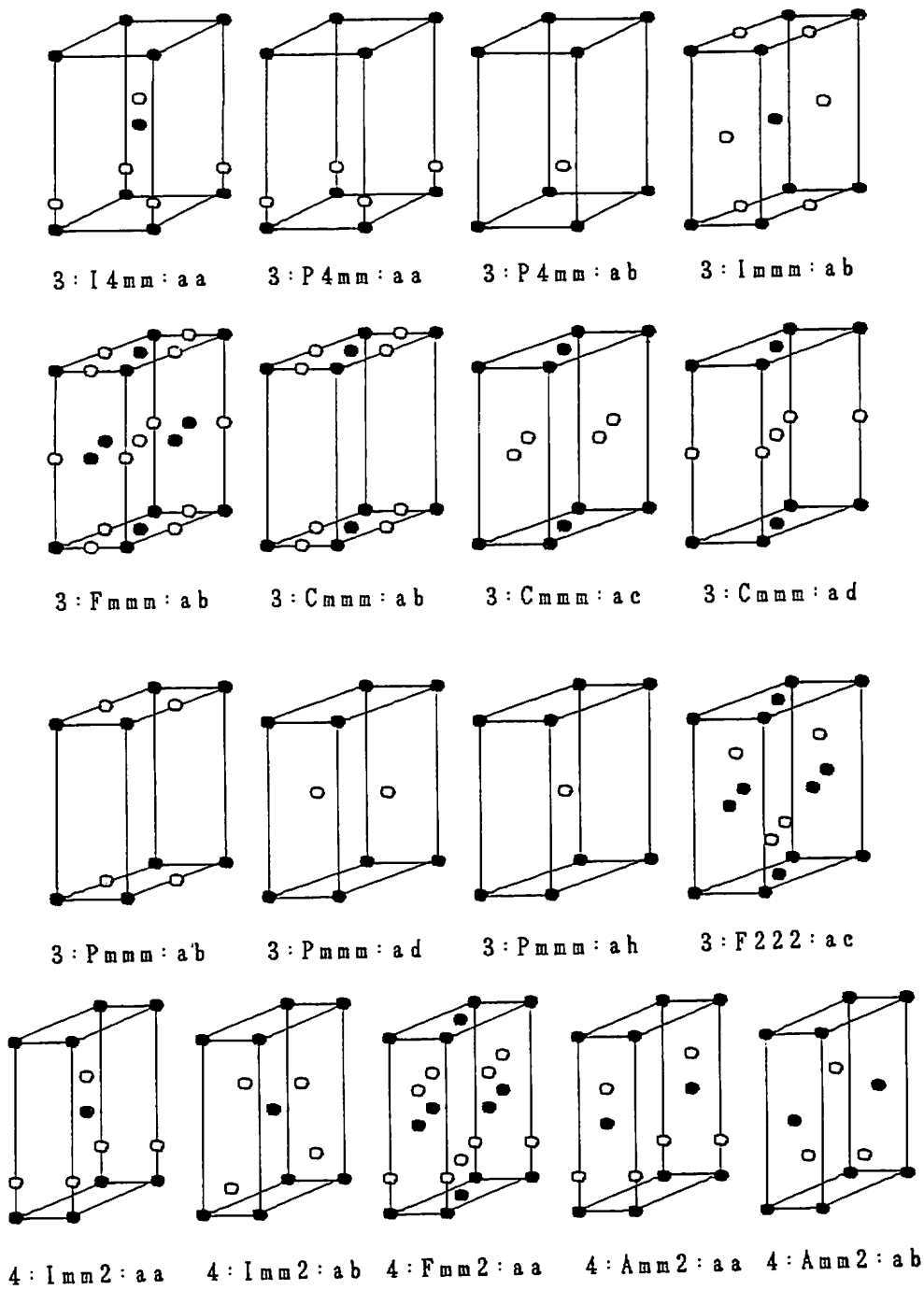

Figure 2. Atomic arrangement of species in genus AB. (Continued)

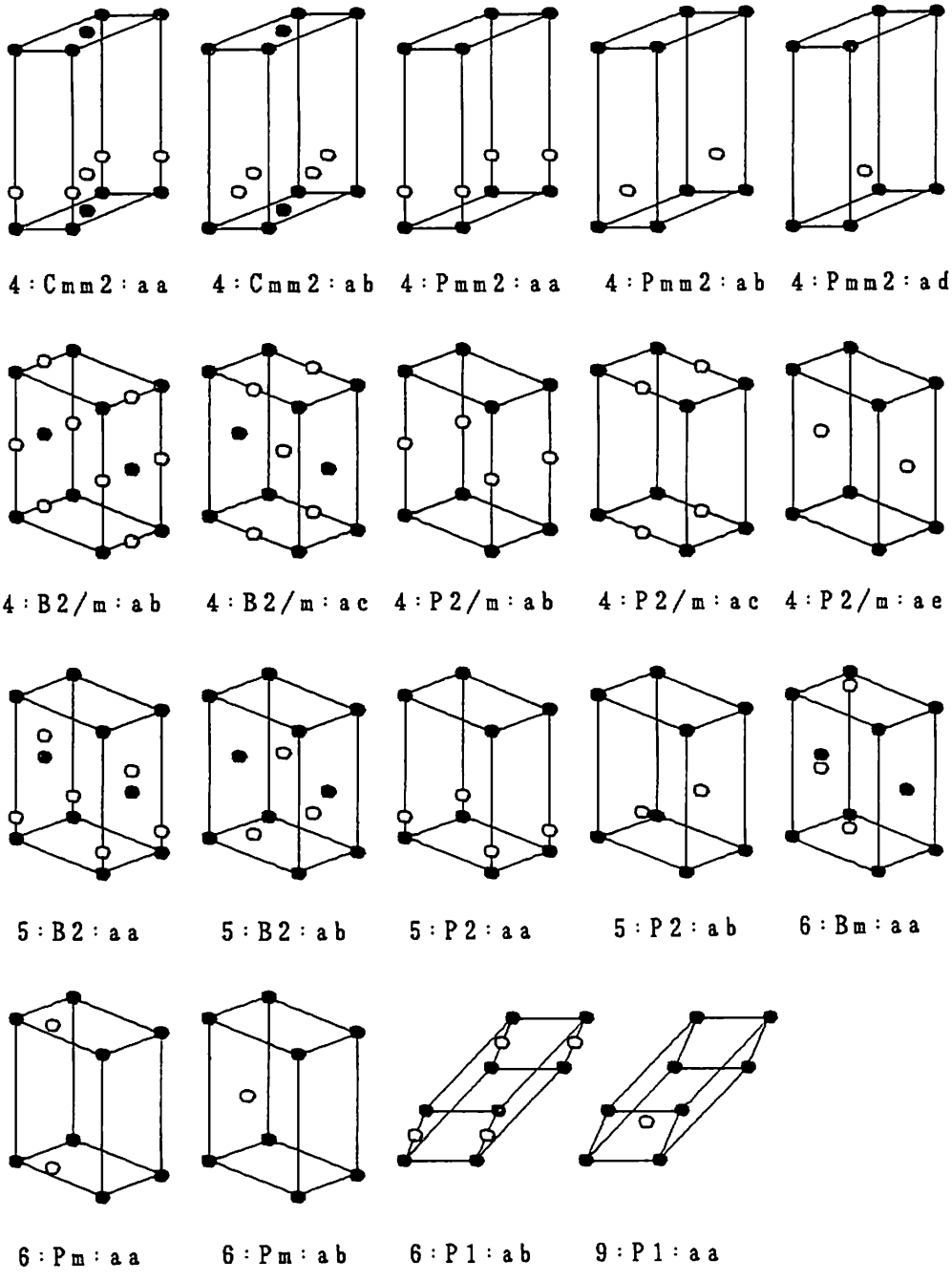

Figure 2. Atomic arrangement of species in genus AB. (Continued)

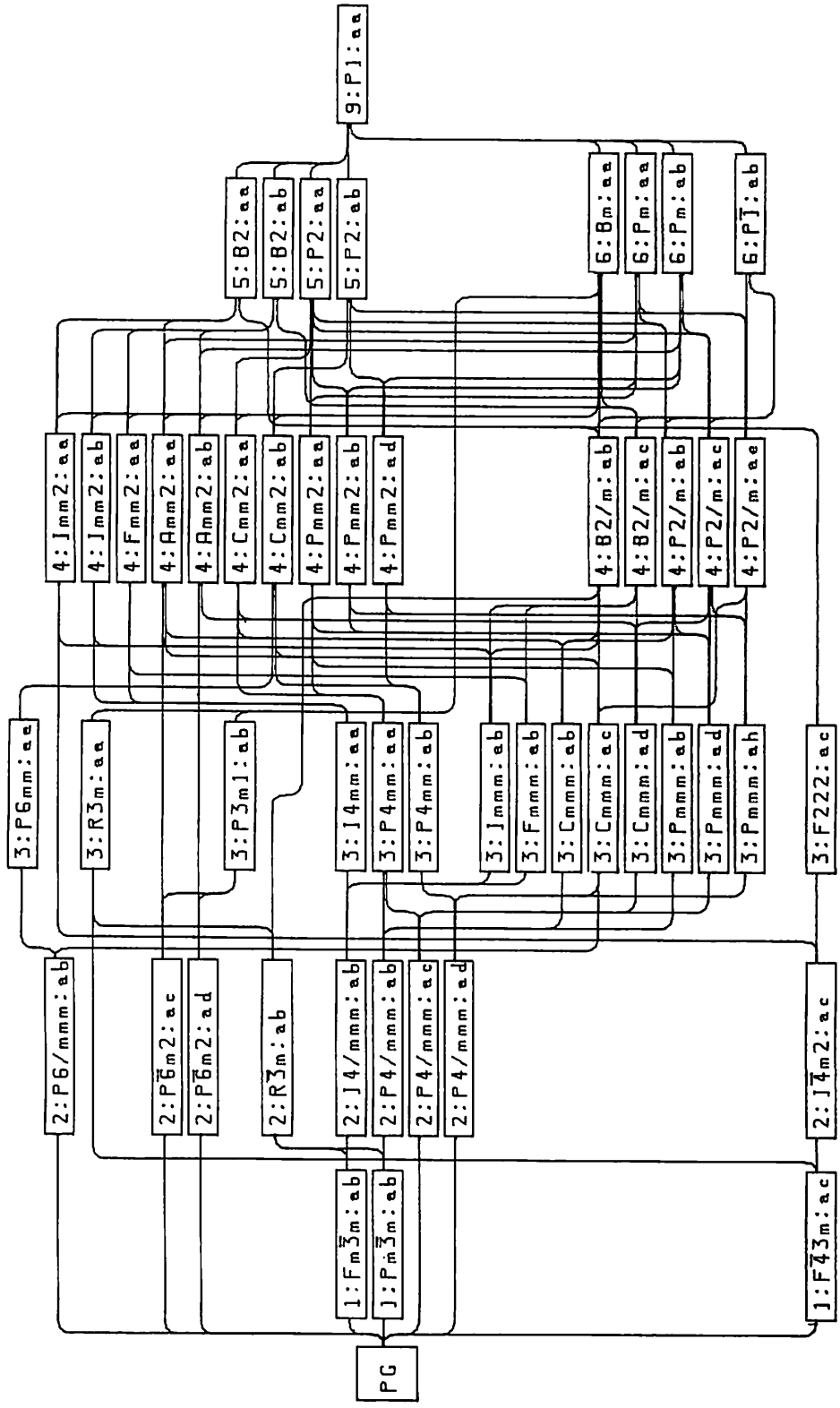

Figure 3. Hierarchy of the species in genus AB. PG means the prototypic group. (Connections are valid only along the rounded corners.)

each other directly, the righthand species is the maximal subgroup of the lefthand one.

IV. Family of Crystal-Structure Types

We complete our classification system by setting up families above genuses. (Hereafter our present system is made differently from that of the author's previous papers (Hosoya, 1980; Hosoya, 1982a; Hosoya, 1982b; Hosoya, 1983).) A family is constructed of all the genuses which have the same number of constituent atoms in their chemical formulas. These numbers will be used as the name of the families. For example family 2 is construcred of genus AB and A_2.

There is a group-subgroup relation between the prototypic groups of the genuses in the same family. For instance the prototypic group of genus AB_2 is a supergroup of that of genus ABC, for the former is obtained by the equalization of atoms B and C in the latter. Thus if we start from the genus such as ABCDE . . . where no letters appear more than once, we can exhaust all the genuses in the family by equalizing the atoms successively.

However such a procedure requires the following consideration. When two genuses $A_\alpha B_\beta C_\gamma$ . . . and $A'_\alpha B'_\beta C'_\gamma$ . . . have the relation $(A'_\alpha B'_\beta C'_\gamma \ldots)_n = A_{\alpha'} B_{\beta'} C_{\gamma'} \ldots$, where n is an integer other than unity, the former will be called the **factor genus** of the latter, and the latter the **multiple genus** of the former. Especially genus $A_\alpha B_\beta C_\gamma$ . . . will be called a **prime factor genus**, if the suffixes α, β, γ, . . . have no common factor other than unity. If a genus is not a prime factor genus, its bpc often degenerates into that of some factor genus. For example 1:Pm3m:ab in genus AB (CsCl structure) is changed into genus A instead of A_2 by equalizing atom A and B. Such a degeneration will be investigated closely in the next section.

V. Interfamily Relations

If a bpc (a, b, c, x_1, x_2, . . .) is given, its corresponding species is uniquely determined. When the bpc is slightly changed, it will be assigned to another species in general. Such a change of species is not always restricted within the genus. As is well known in studies of phase transition, a slight change of atomic position often multiplies the size of the primitive cell. In other words the contents per primitive cell are multiplied. For example, if in a body-centered cubic lattice the atoms at body-center shift to any direction, the size of the primitive cell is doubled, and so is the number of atoms per primitive cell. Since the contents of primitive cell is altered, such a transition accompanies the change of genus. In this section we treat such cell-multiplication or cell-division with the genuses which are transformed to each other by this process. Only the term "cell-division" will be used hereafter because of the convenience stated later, and cell-multiplication will be described as its reciprocal process.

The transition between different genuses occurs because the primitive cell of the multiple genus are divided into the several primitive cells of the factor genus. This process can be straightfowardly handled as the change of bpc of the multiple genus, while the bpc of the factor genus lacks the degree of freedom to express the process. Even the reciprocal process requires the expanded primitive cell different from usual one. Thus the multiple genus and cell-division

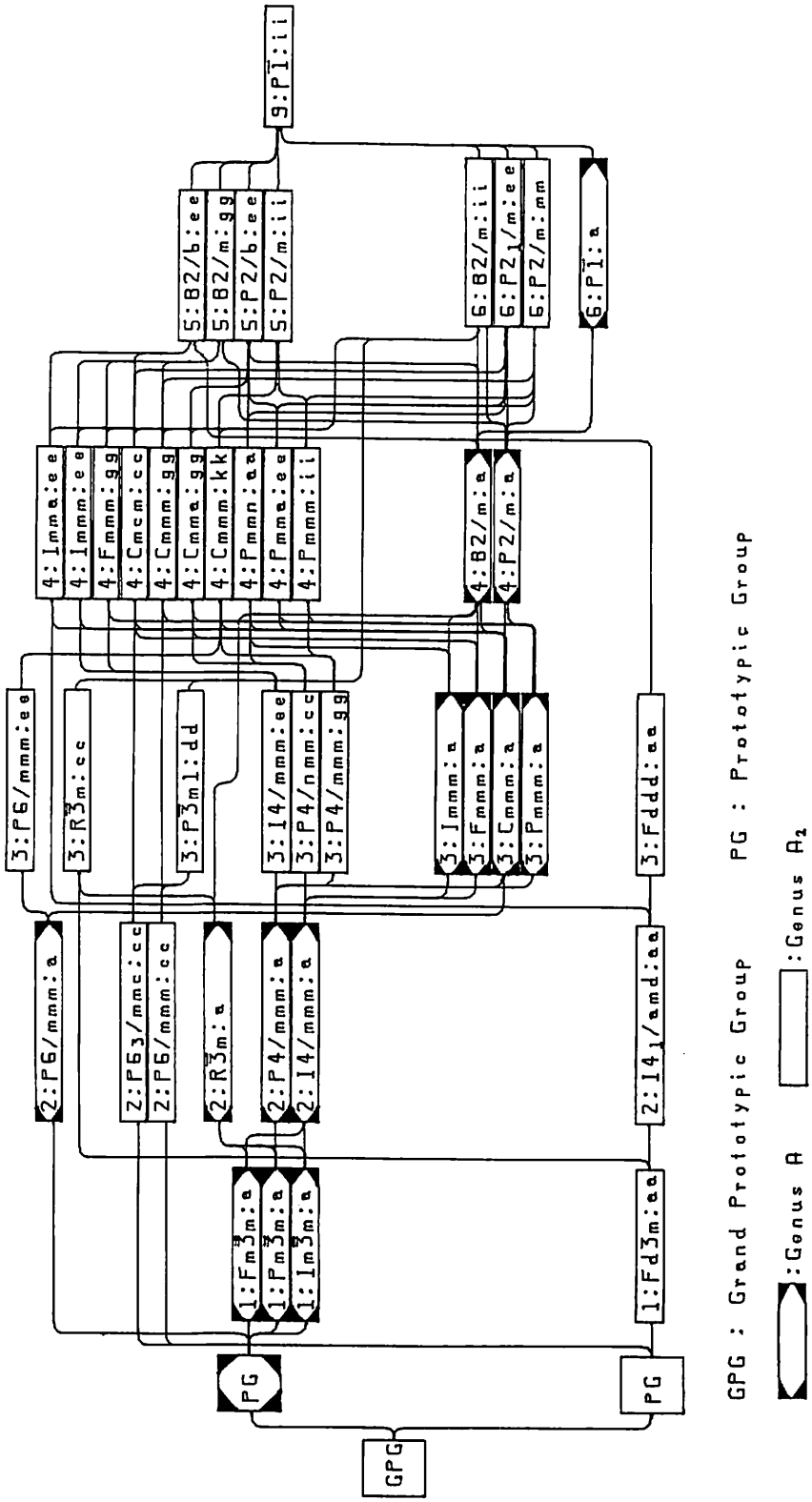

Figure 4. Hierarchy of the species in genus A and A_2.
(Connections are valid only along the rounded corners.)

are principal in such transformations.

If the bpc of a genus degenerates into that of the factor genus, the true primitive translation vectors are not a, b, c, but divided ones of them. Then the components of the transformation matrix of bpc may be the divided integers in the similar way. For example, in genus A_2 the components may be a half-integer or its multiple, when the bpc has changed into that of genus A. In general the transformation matrix may have the following form.

$$\begin{pmatrix} a' \\ b' \\ c' \\ x'_1 \\ \vdots \\ x'_n \end{pmatrix} = \left(\begin{array}{c|c} \text{rational} & 0 \\ \text{unimodular} & 0 \\ & 0 \\ \hline \text{rational} & \text{permutation} \end{array}\right) \begin{pmatrix} a \\ b \\ c \\ x_1 \\ \vdots \\ x_n \end{pmatrix}. \tag{10}$$

(The upper left rational unimodular part of the transformation matrix is a more restricted one than used in defining geometric crystal class Q (Neubüser, Wondratschek & Bülow, 1971).)

In section II, we have assumed that the vectors a, b, c of bpc remain the true primitive

Table 2. Correspondence of species in genus AB to those in A_2 and A.

genus AB	genus A_2	genus A
1 : $Fm\bar{3}m$: ab (NaCl)		1 : $Pm\bar{3}m$: a (s. c.)
1 : $Pm\bar{3}m$: ab (CsCl)		1 : $Im\bar{3}m$: a (b. c. c.)
1 : $F\bar{4}3m$: ac (zinc-blende)	1 : Fd3m : aa (diamond)	
2 : P6/mmm : ab		2 : P6/mmm : a
2 : $P\bar{6}m2$: ac	2 : P6/mmm : cc (honeycomb)	
2 : $P\bar{6}m2$: ad	2 : $P6_3/mmc$: cc (h. c. p.*)	
2 : $R\bar{3}m$: ab		2 : $R\bar{3}m$: a
2 : I4/mmm : ab 2 : P4/mmm : ab 2 : P4/mmm : ac		2 : P4/mmm : a
2 : P4/mmm : ad		2 : I4/mmm : a
2 : $I\bar{4}m2$: ac	2 : $I4_1/amd$: aa	
3 : P6mm : aa	3 : $P6_3/mmm$: ee	
3 : R3m : aa	3 : $R\bar{3}m$: cc	
3 : P3m1 : ab	3 : $P\bar{3}m1$: dd	
3 : I4mm : aa	3 : I4/mmm : ee	
3 : P4mm : aa	3 : P4/mmm : gg	
3 : P4mm : ab	3 : $P4/nmm$: cc	
3 : Immm : ab 3 : Cmmm : ad 3 : Pmmm : ad		3 : Cmmm : a
3 : Fmmm : ab 3 : Cmmm : ab 3 : Pmmm : ab		3 : Pmmm : a
3 : Cmmm : ac		3 : Fmmm : a

genus AB	genus A_2	genus A
3 : Pmmm : ah		3 : Immm : a
3 : F222 : ac	3 : Fddd : aa	
4 : Imm2 : aa	4 : Immm : ee	
4 : Imm2 : ab	4 : Imma : ee	
4 : Fmm2 : aa	4 : Fmmm : gg	
4 : Amm2 : aa	4 : Cmmm : gg	
4 : Amm2 : ab	4 : Cmcm : cc	
4 : Cmm2 : aa	4 : Cmmm : kk	
4 : Cmm2 : ab	4 : Cmma : gg	
4 : Pmm2 : aa	4 : Pmmm : ii	
4 : Pmm2 : ab	4 : Pmma : ee	
4 : Pmm2 : ad	4 : Pmmn : aa	
4 : B2/m : ab 4 : P2/m : ab 4 : P2/m : ac		4 : P2/m : a
4 : B2/m : ac 4 : P2/m : ae		
5 : B2 : aa	5 : B2/m : gg	
5 : B2 : ab	5 : B2/b : ee	
5 : P2 : aa	5 : P2/m : ii	
5 : P2 : ab	5 : P2/b : ee	
6 : Bm : aa	6 : B2/m : ii	
6 : Pm : aa	6 : P2/m : mm	
6 : Pm : ab	6 : $P2_1/m$: ee	
6 : $P\bar{1}$: ab		6 : $P\bar{1}$: a
9 : P1 : aa	9 : $P\bar{1}$: ii	

* The c/a ratio is arbitrary.

translation vectors, and the prototopic group of a genus has been constructed to keep this condition. Therefore the prototypic group in this definition does not contain the translation of fractional a, b, c. Then let us define a new prototypic group of a genus which includes all the operations of the factor genus as well as those of itself, and call it a **grand prototypic group**. A prototypic group in the original definition will be called an ordinary prototypic group or simply a prototypic group. A grand prototypic group contains the ordinary prototypic group of the same genus and both of the grand and ordinary prototypic groups of the factor genuses.

As an example all the species of genus A_2 and A are shown in Figure 4, where the grand prototypic group of A_2 contains every species as its subgroup. The structures of species in genus A_2 are easily obtained by the corresponding species in genus AB by ignoring the difference between atom A and B. This equalization reduces the other species in genus AB to those in genus A. Only the species 1:Fm3m:à (f.c.c.) in genus A is not obtained by this process. The

Table 3. Summary of the classification table of crystal structures.

family	genus	species
1	A	f. c. c., b. c. c., ... (14)
2	AB	NaCl, CsCl, zinc-blende, ... (51)
	A_2	diamond, h. c. p*, ... (29)
3	ABC	.....
	AB_2	fluorite, ...
	A_3	.....
4	ABCD	.....
	ABC_2	.....
	AB_3	BiF_3, ReO_3, ...
	A_2B_2	NaTl, NiAs, wurtzite, ...
	A_4	.....
5	ABCDE	.....
	$ABCD_2$	.....
	ABC_3	perovskite, ...
	AB_2C_2	.....
	AB_4	.....
	A_2B_3	.....
	A_5	.....
6		

* The c/a ratio is arbitrary.

correspondence of species in genus AB to those in A_2 and A is shown in Table 2.

VI. Summary and Discussion

Any crystal-structure type has the corresponding structure group which has been newly defined in the present paper. It is classified into a species, genus, and family successively. For example NaCl structure belongs to species 1:Fm$\bar{3}$m:ab, genus AB, and family 2. If the species and genus are given, the family is self-evident. So we will only use the species and genus as the name of crystal-structure type. The summary of the classification system is shown in Table 3.

Instead of a structure group, we can also use the bpc (a, b, c, x_1, x_2, . . .) to indicate the species. The bpc is far more convenient for us to grasp the geometrical meaning of the species. However, the criterion whether any two crystal-structure types are equivalent or not can not be given without the use of their structure groups. Most of the previous works seem to have concerned only the bpc or some similar objects.

References

AIZU, K. (1962). *Rev. mod. Phys.* 34, 550-576.

AIZU, K. (1966). *Phys. Rev.* 146, 423-429.

AIZU, K. (1969). *J. Phys. Soc. Jpn.* 27, 387-396.

AIZU, K. (1970). *Phys. Rev.*B2, 754-772.

AIZU, K. (1979). *J. Phys. Soc. Jpn.* 46, 1716-1725.

BRADLEY, C. J. & CRACKNELL, A. P. (1972). *The Mathematical Theory of Symmetry in Solids*, p.95. Clarendon Press.

HOSOYA, M. (1979). J. Phys. Soc. Jpn. 46, 1691-1694, errata in *J. Phys. Soc. Jpn.* 47, (1979) 1732.

HOSOYA, M. (1980). *Bussei Kenkyu* 34, 297-313 (in Japanese)

HOSOYA, M. (1982a). *Bull. Coll. Sci. Univ.* Ryukyus 33, 9-26. (in Japanese)

HOSOYA, M. (1982b). *Bull. Coll. Sci. Univ. Ryukyus* 34, 1-73. (in Japanese)

HOSOYA, M. (1983). *Bull. Coll. Sci. Univ. Ryukyus* 35, 9-52. (in Japanese)

NEUBÜSER, J., WONDRATSCHEK, H. & BÜLOW, R. (1971). *Acta Cryst.* 27A, 517-520, 520-523, 523-535.

NIGGLI, A. (1971). *Z. Kristallogr.* 133, 473-490.

SAKAMOTO, Y. (1974). *J. Sci. Hiroshima Univ., Ser. A* 38, 239-270.

SAKAMOTO, Y., KIDA, A., HIRAGA, K. & MURATA, H (1983). *J. Sci. Hiroshima Univ.*, Ser. A 46, 371-461.