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# A finite group that derives all the 14 Bravais lattices as its subgroups

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A finite group was discovered that includes all the types of Bravais lattice as its subgroups. It is based on a new representation of affine transformation of a primitive cell. Its elements are represented by  $6 \times 6$  matrices whose components are complex in general. The order of the group is 2799360.

1. Introduction

Like other entities in crystallography, each type of Bravais lattice has its corresponding group (Burckhardt, 1966; Schwarzenberger, 1972, 1974; Neubüser et al., 1971; Wondratschek et al., 1971; Bülow et al., 1971; Hosoya, 1979). The well known 14 types are connected to each other by group-subgroup relations as shown in Fig. 1 (Hosoya, 1979). Since all the 14 types are also connected to a supergroup, they can be regarded as the result of symmetry breakdown, which is brought about by the occurrence of certain irreducible representations in the supergroup. Such a consideration tempts us to apply a phenomenological theory like Landau's (Landau & Lifshitz, 1962; Aizu, 1962, 1966, 1970; Hosoya, 1977) to all the phase transitions that accompany a change of Bravais-lattice type. However, the supergroup is infinite, which often makes our attempts impossible. For example, the phase transitions of solid iron cannot be treated by the Landau theory because it needs a finite supergroup of body-centered cubic (b.c.c.) and face-centered cubic (f.c.c.). If we find a finite supergroup that keeps the interrelations among its subgroups, the above plan becomes feasible. The present paper gives such a finite supergroup.

#### 2. Generators of affine mapping

A Bravais lattice is algebraically defined as a group of affine mappings, each of which maps its lattice onto itself and can also be realized by a point symmetry operation (Burckhardt, 1966; Schwarzenberger, 1972, 1974). For example, when the primitive cell vectors are given as  $\mathbf{a} = (x, 0, 0)$ ,  $\mathbf{b} = (x/2, 3^{1/2}x/2, 0)$ ,  $\mathbf{c} = (0, 0, z)$ , where x and z are arbitrary, the sixfold rotation about the c axis to  $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$  is represented by the following affine mapping:

$$\begin{pmatrix} \mathbf{a}' \\ \mathbf{b}' \\ \mathbf{c}' \end{pmatrix} = \begin{pmatrix} 1 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{pmatrix}.$$
 (1)

On the other hand, it can also be realized by each point operation of **a**, **b** and **c** such as

$$\begin{pmatrix} \mathbf{a}'_x \\ \mathbf{a}'_y \\ \mathbf{a}'_z \end{pmatrix} = \begin{pmatrix} 1/2 & 3^{1/2}/2 & 0 \\ -3^{1/2}/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{a}_x \\ \mathbf{a}_y \\ \mathbf{a}_z \end{pmatrix}.$$
 (2)

If we decompose the set of basis (**a**, **b**, **c**) into a nine-dimensional vector ( $a_x$ ,  $a_y$ ,  $a_z$ ,  $b_x$ ,  $b_y$ ,  $b_z$ ,  $c_x$ ,  $c_y$ ,  $c_z$ ) and consider each component of the matrix of affine transformation as a 3 × 3 matrix, we can show the above relation explicitly as follows:



In general, we may describe such relations symbolically as

$$\mathbf{A}\begin{pmatrix}\mathbf{a}\\\mathbf{b}\\\mathbf{c}\end{pmatrix} = \mathbf{O}\begin{pmatrix}\mathbf{a}\\\mathbf{b}\\\mathbf{c}\end{pmatrix},\tag{4}$$

Table 1

Groups corresponding to Bravais lattices with the highest symmetry.					
Group	Lattice basis	Generators	Order		
Simple cubic <b>G</b> <sub>sc</sub>	$(x_1, 0, 0; 0, x_1, 0; 0, 0, x_1)$	$(C_{2b}, C_{31+}, C_{47+}, I)$	48		
Body-centered cubic G <sub>bcc1</sub>	$(-x_2, x_2, x_2; x_2, -x_2, x_2; x_2, x_2, -x_2)$	$(C_{2b}, C_{31+}, {}^{b}C_{47+}, I)$	48		
Body-centered cubic $G_{hcc2}$	$(x_3, x_3, x_3; x_3, -x_3, x_3; 2x_3, 0, 0)$	$(C_{2b}, {}^{b}C_{31+}, {}^{f}C_{47+}, I)$	48		
Face-centered cubic G <sub>fcc</sub>	$(0, x_4, x_4; x_4, 0, x_4; x_4, x_4, 0)$	$(C_{2b}, C_{31+}, {}^{f}C_{47+}, I)$	48		
Hexagonal G <sub>hex</sub>	$(x_5, 0, 0; x_5/2, 3^{1/2}x_5/2, 0; 0, 0, x_6)$	$(C_{2b}, C_{6+}, I)$	24		

where **A** and **O** are the affine and the orthogonal (rotational) transformation, respectively. The group of a Bravais lattice is a set of left-hand operations that satisfy equation (4). Such an affine operation is represented by a  $3 \times 3$  integral unimodular matrix (Burckhardt, 1966; Neubüser *et al.*, 1971). The types of two Bravais lattice are distinguished according to whether they are inner automorphic to each other in the group of all the integral unimodular matrices (Hosoya, 1979). Since the right-hand operations of equation (4) constitute one of the crystal point groups, the group of the Bravais lattice is isomorphic to it.

In order to identify the 14 Bravais types, only the following generators are needed.

$$C_{2b} = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad C_{31+} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

$$C_{4z+} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad {}^{b}C_{4z+} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix},$$

$${}^{f}C_{4z+} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & -1 \\ -1 & 1 & 0 \end{pmatrix}, \qquad {}^{b}C_{31+} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & -1 \\ 1 & 1 & -1 \end{pmatrix},$$

$$C_{6+} = \begin{pmatrix} 1 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad I = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$
(5)

Here their labels are named from Jones's faithful representation symbols for their corresponding symmetry operations of the point group (Bradley & Cracknell, 1972). The additional superscripts b and f indicate a body-centered cell and a face-centered one, respectively. The geometrical meaning of  $C_{2b}$ ,  $C_{31+}$ ,  $C_{4z+}$ ,  $C_{6+}$  and I may be easily obtained, since each of them shows a literal operation when  $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ represents a unit cell of a simple cubic or hexagonal lattice. The meaning of  ${}^{b}C_{4z+}$ ,  ${}^{f}C_{4z+}$  and  ${}^{b}C_{31+}$  becomes clear if we take their conventional-cell vectors  $(\mathbf{i}, \mathbf{j}, \mathbf{k})$  as

$$\mathbf{i} = \mathbf{b} + \mathbf{c}, \quad \mathbf{j} = \mathbf{c} + \mathbf{a}, \quad \mathbf{k} = \mathbf{a} + \mathbf{b};$$
 (6)

$$\mathbf{i} = -\mathbf{a} + \mathbf{b} + \mathbf{c}, \quad \mathbf{j} = \mathbf{a} - \mathbf{b} + \mathbf{c}, \quad \mathbf{k} = \mathbf{a} + \mathbf{b} - \mathbf{c};$$
 (7)

$$i = c, j = a - b, k = a + b - c;$$
 (8)

respectively. The labels have an appropriate meaning with respect to the transformation of  $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ . For example,  ${}^{b}C_{4z+}$ 

corresponds to a fourfold rotation about the k axis in (6), where (**i**, **j**, **k**) represents a set of conventional-cell vectors of a body-centered lattice.

Among the 14 Bravais types, the hexagonal group and the three cubic ones have the highest symmetry and contain all the other groups as their subgroup. Then we might have only to find a minimal supergroup of these

four groups. However, there is a special situation as to the cubic groups. No pair of body-centered cubic group and facecentered cubic group share a rhombohedral group and a bodycentered tetragonal group at the same time. (See Fig. 2.) In Fig. 1, face-centered cubic and body-centered cubic groups seem to have rhombohedral and body-centered tetragonal groups simultaneously. However, every entry in the figure represents all the equivalent groups, and not a particular one. Hence, face-centered cubic and body-centered cubic groups should not be regarded as two particular groups but representative of all the corresponding equivalent groups. For the supergroup to constitute a complete system, it must not only contain all the subgroups but deduce the same groupsubgroup relations among them. Accordingly, we must prepare at least two types of b.c.c. or f.c.c. as our foothold. We choose the most convenient set of groups as in Table 1, where  $G_{sc}$ ,  $G_{bcc1}$  and  $G_{fcc}$  include the rhombohedral group with order 12 generated by  $(C_{2b}, C_{31+}, I)$  in common, while  $\mathbf{G}_{bcc2}$  and  $\mathbf{G}_{fcc}$ share the body-centered tetragonal group with order 16 generated by  $(C_{2b}, {}^{f}C_{4z+}, I)$ .

Order



Figure 1 Hierarchy of the 14 Bravais lattices.

#### 3. A new representation

Now we try to change the operators to make their set close within a finite order. After the change, the relations between the elements must be kept for the same group–subgroup relations to hold between the 14 Bravais types. We must first choose another representation of their elements. In a previous paper, the author gave a simple method to define the mapping of a lattice onto itself (Hosoya, 1979). It uses a 'primitive tetrahedron', which has its four corners at some lattice points and contains none within it. The tetrahedron is specified by a six-dimensional vector (a, b, c, p, q, r) whose elements are the length of its six edges. They are easily given from a set of independent primitive translation vectors **a**, **b**, **c** as follows:

$$a = |\mathbf{a}|, \ b = |\mathbf{b}|, \ c = |\mathbf{c}|,$$
$$p = |\mathbf{b} - \mathbf{c}|, \ q = |\mathbf{c} - \mathbf{a}|, \ r = |\mathbf{a} - \mathbf{b}|.$$
(9)

[The present definition is different from that of Hosoya (1979).] This definition, however, gives only positive values to all the components and therefore cannot distinguish a primitive cell  $(\mathbf{a}, \mathbf{b}, \mathbf{c})$  from its inverted one  $(-\mathbf{a}, -\mathbf{b}, -\mathbf{c})$ . In general, we cannot discriminate a cell from its enantiomorph in terms of the present representation. Accordingly, any symmetry operation that transforms a cell into its enantiomorphic one also reduces into the corresponding proper operation. For example, both inversion and reflection become the identity operation, while an improper rotation like  $S_3$  becomes a proper rotation such as  $C_3$ . The order of every group in Fig. 1 becomes half as much as the original one. However, this is not a fatal fault, for any Bravais lattice has an inversion symmetry by nature and its essential six parameters can be determined only by proper operations.

Using these relations, the generators of equation (5) can be translated into those that transform a vector (a, b, c, p, q, r) as follows. (Hereafter, we represent each vector as a row to save space.)

$$C_{2b}(a, b, c, p, q, r) = (b, a, c, q, p, r)$$
(10)

$$C_{31+}(a, b, c, p, q, r) = (c, a, b, r, p, q)$$
(11)

$$C_{4z+}(a, b, c, p, q, r) = (b, a, c, q, \{2[b^2 + c^2] - p^2\}^{1/2},$$

$$\{2[a^{2}+b^{2}]-r^{2}\}^{1/2}\}$$
(12)  
<sup>b</sup>C<sub>4z+</sub>(a, b, c, p, q, r) = (\{3[a^{2}+b^{2}+c^{2}]-p^{2}-q^{2}-r^{2}\}^{1/2}, c, a, q,   

$$\{4[2a^{2}+b^{2}+c^{2}]-p^{2}-2a^{2}-2r^{2}\}^{1/2}$$

$$\{4[a^2 + b^2 + 2c^2] - 2p^2 - 2q^2 - r^2\}^{1/2}) \quad (13)$$

$${}^{f}C_{4z+}(a, b, c, p, q, r) = (b, p, r, q, a, c)$$
(14)

$${}^{b}C_{31+}(a, b, c, p, q, r) = (a, q, [a^{2} + b^{2} - c^{2} + p^{2} + q^{2} - r^{2}]^{1/2}, b, p, c)$$
(15)

$$C_{6+}(a, b, c, p, q, r) = (r, a, c, q, [b^2 + c^2 - a^2 + q^2 + r^2 - p^2]^{1/2}, b)$$

(16)  
$$I(a, b, c, p, q, r) = (a, b, c, p, q, r).$$
 (17)

A great advantage of this representation exists in that the corresponding equation to (4) is simplified as follows:

$$\mathbf{A}(a, b, c, p, q, r) = (a, b, c, p, q, r).$$
(18)

Thus, a group of Bravais lattices corresponds to that of affine transformations that keep the primitive tetrahedron invariant.

#### 4. Linearization of generators

Since the above generators contain nonlinear transformations, they cannot be represented by a matrix in general. Let us change the nonlinear operators  $C_{4z+}$ ,  ${}^{b}C_{4z+}$ ,  ${}^{b}C_{31+}$  and  $C_{6+}$  into  ${}^{l}C_{4z+}$ ,  ${}^{lb}C_{4z+}$ ,  ${}^{lb}C_{31+}$  and  ${}^{l}C_{6+}$ , respectively, where the superscripts *l* mean 'linearized'.

$${}^{l}C_{4z+}(a, b, c, p, q, r) = (b, a, c, -q, p, -r)$$
(19)

$${}^{lb}C_{4z+}(a, b, c, p, q, r) = (-b, a, -c, q, p, r)$$
(20)

$${}^{lb}C_{31+}(a, b, c, p, q, r) = (a, q, c \exp[i2\pi/3], b, p, r \exp[-i2\pi/3])$$
(21)

$${}^{l}C_{6+}(a, b, c, p, q, r) = (r, a, c, p \exp[i\pi/3], q \exp[-i\pi/3], b).$$
(22)

Operators  ${}^{l}C_{4z+}$  and  ${}^{lb}C_{4z+}$  were straightforwardly found because they have a cycle with order 4.  ${}^{lb}C_{31+}$  and  ${}^{l}C_{6+}$  were also directly suggested by the fact that they are cyclic with order 3 and 6 in the space (c, r) and (p, q), respectively. These operators are, of cource, not unique, but may have a number of equivalents. However, they have been deliberately chosen after several trials so that new figures such as  $\exp(i\pi/3)$  or  $\exp(i2\pi/3)$  should be as few as possible, since they inevitably generate new elements that increase the order of the minimal supergroup. For example,  ${}^{l}C_{4z+}$  is defined without using  $\exp(i2\pi/4)$ .

Then we choose the bases and the generators of the alternate five groups as in Table 2. It should be noticed that no



Hierarchy of the newly obtained groups.

Table 2

L	inearized	groups	corresponding	to	Bravais	lattices	with	the	highest	symn	netry
		<u> </u>	1 0						<u> </u>	~	~

Group	Lattice basis	Generators	Order
Simple cubic <sup>1</sup> G <sub>sc</sub>	$(x_1, x_1, x_1, 0, 0, 0)$	$(C_{2b}, C_{31+}, {}^{l}C_{47+})$	24
Body-centered cubic <sup>1</sup> G <sub>bcc1</sub>	$(0, 0, 0, x_2, x_2, x_2)$	$(C_{2b}, C_{31+}, {}^{lb}C_{47+})$	24
Body-centered cubic <sup>1</sup> G <sub>bcc2</sub>	$(x_3, x_3, 0, x_3, x_3, 0)$	$(C_{2b}^{a}, {}^{lb}C_{31+}, {}^{f}C_{47+})$	24
Face-centered cubic G <sub>fcc</sub>	$(x_4, x_4, x_4, x_4, x_4, x_4, x_4)$	$(C_{2b}, C_{31+}, {}^{f}C_{4z+})$	24
Hexagonal <sup>1</sup> G <sub>hex</sub>	$(x_5, x_5, x_6, 0, 0, x_5)$	$(C_{2b}, {}^{l}C_{6+})$	12

linearization is necessary for the face-centered cubic  $G_{fcc}$ . Each of these groups has the same structure as its original one.

#### 5. Results

Now all the generators can be represented by  $6 \times 6$  matrices. Every generator is a monomial matrix, which is defined as one having nonzero components once and only once in each row and column, and any product of such matrices becomes also a monomial one. So every matrix of the group must be a monomial one whose configuration of nonzero components takes one of 6! possibilities. Furthermore, the value of the nonzero component is one of the following six figures: 1,  $\exp(i\pi/3)$ ,  $\exp(i2\pi/3)$ , -1,  $\exp(-i2\pi/3)$ ,  $\exp(-i\pi/3)$ . Therefore, the group generated by these matrices is finite and its order never exceeds  $6! \times 6^6 = 33\,592\,320$ .

With the help of computers, all the generators were multiplied by each other successively until no new element appeared. Programs were written in Basic (F-Basic V6.0 L10 provided by Fujitsu) by the author and used mainly on a personal computer GP6-333 provided by Gateway 2000. The results are shown in Fig. 2. The supergroup  $G_0$  with 2799360 elements is our final goal whose computation took about one week and needed a data file of 17 Mbytes on a hard disk. Five intermediate subgroups from  $G_1$  to  $G_5$  were found that contain some of the five foothold groups simultaneously. All the six groups are determined as the minimal supergroup produced by the generators of their corresponding subgroups. Hence, for example,  $G_1$  and  $G_2$  are distinguished from each other, for the former contains a generator  ${}^{l}C_{6+}$  of  ${}^{l}\mathbf{G}_{hex}$  and the latter does not, while the latter contains  ${}^{lb}C_{31+}$  of  ${}^{l}\mathbf{G}_{bcc2}$  and the former does not.

Our first aim to find a finite supergroup of all the Bravais lattices has been achieved. However, its use as a prototypic group in the Landau theory of phase transitions needs further laborious work. First of all, its irreducible representations must be obtained but even their total number has not been determined yet. No complete analysis of  $G_0$ , however, is necessary in particular cases. For example, phase transitions of solid iron need a supergroup of only b.c.c. and f.c.c. so that  $G_3$ or  $G_4$  is sufficient. Since their analyses are far simpler than that of  $G_0$ , we will be able to treat such transitions very soon.

The present results and methods will offer convenience to crystallography. Above all, a finite supergroup simplifies the enumeration of its subgroups. For example, the 32 crystalsponding latter one and the group  $C_i$  consisting of elements (E, I), where E is the identity element and I is

$$I = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}.$$
 (23)

lographic point groups have quite similar group–subgroup relations under the two most symmetrical groups 6/mmm and m3m to those under  ${}^{1}\textbf{G}_{hex}$  and  ${}^{1}\textbf{G}_{sc}$  in Fig. 2. Groups 6/mmm and m3m are homomorphic to  ${}^{1}\textbf{G}_{hex}$  and  ${}^{1}\textbf{G}_{sc}$ , respectively, with two-to-one correspondence. Each of the former two groups can be constructed as the direct product of the corre-

Thus, all the crystallographic point groups may be deduced as the subgroups of  $G_1$ , which has been found to contain the above *I*. [It should be noticed that the present *I* is not a sixdimensional version of inversion given in equation (5), but a somewhat artificial one newly introduced.]

The most important usefulness of the present result lies in the fact that many problems become solvable with algebraic methods, which means more automatic methods than geometric ones. An example may be the determination of the reduced basis of lattices, that is the necessary and sufficient region to represent all the possible Bravais lattices in their parameter space (Hosoya, 1986, 1990). Group theoretically, the basis is a fundamental region of the representation space for the infinite supergroup of all the Bravais lattices. Since most of the elements are nonlinear, no systematic method is applicable to obtain it. Only a careful geometrical survey could give the answer. Now all the elements of the supergroup have become linear, the region will be gained almost automatically. Since the components of the elements are complex in general, the obtained region will be also complex. Then the region must be translated into the original representation space, which is not so difficult a task.

The author expects that the present method is applicable to higher-dimensional crystallography because there seems to be no essential difficulty in its expansion but much closer investigation will be necessary.

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## addenda and errata

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## addenda and errata

### A finite group that derives all the 14 Bravais lattices as its subgroups. Erratum

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There is a mistake in Fig. 2 of the paper by Hosoya [*Acta Cryst.* (2000), A**56**, 259–263]. The line connecting  $G_1$  to  $G_3$  is wrong and should connect  $G_1$  and  $G_5$  as shown in the following figure, which replaces Fig. 2 of the original paper.

The author is grateful to Dr Katsushi Waki for pointing out the error.

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Hosoya, M. (2000). Acta Cryst. A56, 259-263.



Figure 2 Hierarchy of the newly obtained groups.