CLAPP, P. C. & MOSS, S. C. (1968). *Phys. Rev.* **171**, 754–763.
FONTAINE, D. DE (1975). *Acta Metall.* **23**, 533–571.
FONTAINE, D. DE (1981). *Metall. Trans. A*, **12A**, 559–566.
International Tables for X-ray Crystallography (1952). Vol. I. Birmingham: Kynoch Press.
KANAMORI, J. & KAKEHASHI, Y. (1977). *J. Phys. (Paris)*, **38**, C7274–C7279.
KHACHATURYAN, A. G. (1973). *Phys. Status Solidi*, **60**, 9–37.
KUDO, T. & KATSURA, S. (1976). *Prog. Theor. Phys.* **56**, 435–449.
LANDAU, L. D. & LIFSHITZ, E. M. (1958). *Statistical Physics*, p. 386, Reading, Mass.: Addison-Wesley.
MCCONNELL, J. D. C. (1978*a*). *Phys. Chem. Miner.* **2**, 253–265.
MCCONNELL, J. D. C. (1978*b*). *Z. Kristallogr.* **147**, 45–62.
OKAMOTO, P. R. & THOMAS, G. (1971). *Acta Metall.* **19**, 825–841.
RICHARDS, M. J. & CAHN, J. W. (1971). *Acta Metall.* **19**, 1263–1277.
SANCHEZ, J. M. & DE FONTAINE, D. (1981). *Structure and Bonding in Crystals*, Vol. II, edited by M. O'KEEFFE & A. NAVROTSKY. New York: Academic Press. In the press.
SEITZ, F. (1936). *Ann. Math.* **37**, 17–26.
WYCKOFF, R. W. G. (1922). *The Analytical Expression of the Results of the Theory of Space Groups.* The Carnegie Institution, Washington, DC.

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The Subgroups of the Finite Double Point Groups

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Abstract

Theorems referring to subgroups of the finite double point groups are formulated. All possible non-evident subgroups are enumerated. The results obtained for subgroups correspond to well known Opechowski rules for classes of double groups.

For some purposes, *e.g.* for finding the transitive permutational representations (Hall, 1959; Gorzkowski, 1976) playing a very important role in so-called coloured symmetry, it is necessary to know all the subgroups of the finite double point groups. This problem is analyzed in this paper. Three theorems referring to the subgroups of the finite double point groups will be formulated. In a certain sense these theorems are analogous to the well known Opechowski (1940) rules referring to the classes of double point groups.

According to Gorzkowski & Suffczynski (1978) we remark that if H is a subgroup of the single group G, then the double group $\bar{H}$ is a subgroup of the double group $\bar{G}$. This fact is used implicitly in many expositions dealing with the double groups (*e.g.* Bradley & Cracknell, 1972) and it will not be proved here.

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A subgroup of the double point group which itself is a double group in the sense that it includes the identity E and the rotation $\bar{E}$ through the angle 2π shall be called an evident subgroup. The problem of the non-evident subgroups of all the crystallographic double point groups has been solved (Gorzkowski & Suffczynski, 1978). Now the finite double point groups without crystallographic restrictions are investigated.

At the beginning, for simplicity, the double point groups without improper rotations are taken into account. The following theorem will be proved.

Theorem 1

Every non-evident subgroup of the finite double point group without improper rotations can contain only the rotations $\bar{C}^{l}_{n+\frac{1}{2}}$ through the angles $4\pi l/(2n+1)$ where l and n are integers.

Proof. At first the even-order symmetry axis is considered. Let C_{2n} denote the rotation through the angle $2\pi/2n = \pi/n$, and $\bar{C}_{2n}$ the rotation through the angle $\pi/n + 2\pi$. One can have:

$$C^{2n}_{2n} = \bar{C}^{2n}_{2n} = \bar{E}.$$

We see that the group generated by C_{2n} or $\bar{C}_{2n}$ contains both $\bar{E}$ and E. Therefore, the subgroup containing the even-order symmetry axis is an evident one.

Now the odd-order symmetry axis is taken into account. Let C_{2n+1} denote the rotation through the

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angle $2\pi/(2n+1)$ and $\bar{C}_{2n+1}$ the rotation through the angle $2\pi/(2n+1)+2\pi$. Now, we can have:

$$C_{2n+1}^{2n+1}=\bar{E},$$

$$\bar{C}_{2n+1}^{l}\neq\bar{E},\quad \text{for every integer } l.$$

This means that the subgroups generated by C_{2n+1} are evident ones, but the subgroups generated by $\bar{C}_{2n+1}$ are non-evident ones. We have:

$$(C_{2n+1}^{2})^{n+1}=\bar{C}_{2n+1}.$$

Therefore, the subgroup generated by $\bar{C}_{2n+1}$ is also generated by C_{2n+1}^2. The operation C_{2n+1}^2 is the rotation through the angle $2\times 2\pi/(2n+1)=2\pi/(n+\frac{1}{2})$. Owing to this fact we can denote the operation C_{2n+1}^2 by the symbol $C_{n+\frac{1}{2}}$. The elements of the non-evident subgroups considered are the following:

$$E, C_{n+\frac{1}{2}}, C_{n+\frac{1}{2}}^2, C_{n+\frac{1}{2}}^3, C_{n+\frac{1}{2}}^4, \ldots, C_{n+\frac{1}{2}}^l, \ldots.$$

One can now proceed to the finite double point groups with improper rotations. The following theorem will be proved.

Theorem 2

The non-evident double point subgroups can contain only the following operations:

$$C_{n+\frac{1}{2}}^p, (IC_{n+\frac{1}{2}})^q, (\bar{I}C_{n+\frac{1}{2}})^r,$$

where p, q, r and n are integers.

Proof. From the proof of the preceding theorem we know that the non-evident subgroups can contain only the following proper rotations: E, $C_{n+\frac{1}{2}}$, $C_{n+\frac{1}{2}}^2$, ... For completeness, the improper rotations of the form IC_k and $\bar{I}C_k$ should also be considered. In a similar way as before one can see that for even k one can have:

$$(IC_k)^k=(\bar{I}C_k)^k=\bar{E}$$

(I and $\bar{I}$ commute with every C_k).

This means that the non-evident subgroup cannot contain the rotations IC_k or $\bar{I}C_k$ with even k.

Thus, every non-evident subgroup can include only such improper rotations for which k is an odd integer. It denotes that every non-evident subgroup has to be constructed from the operations of the form:

$$C_{n+\frac{1}{2}}^p, (IC_{n+\frac{1}{2}})^q, (\bar{I}C_{n+\frac{1}{2}})^r.$$

Theorem 2 gives all the possible elements of the non-evident subgroups of the finite double point groups. One can now combine these elements in order to find all the non-evident subgroups.

The last theorem will now be proved.

Theorem 3

All the possible non-evident subgroups of the finite double point groups are the following:

$$\bar{C}_{\frac{1}{2}}=\{E\}$$

$$\bar{C}_{\frac{3}{2}}=\{E, C_{\frac{3}{2}}, C_{\frac{3}{2}}^2\}$$

$$\bar{C}_{\frac{5}{2}}=\{E, C_{\frac{5}{2}}, C_{\frac{5}{2}}^2, C_{\frac{5}{2}}^3, C_{\frac{5}{2}}^4\}$$

. . . .

$$\bar{C}_{n+\frac{1}{2}}=\{E, C_{n+\frac{1}{2}}, C_{n+\frac{1}{2}}^2, C_{n+\frac{1}{2}}^3, \ldots, C_{n+\frac{1}{2}}^{2n}\}$$

. . . .

$$\bar{C}_{\frac{1}{2}i}=\{E, I\}$$

$$\bar{C}_{\frac{3}{2}i}=\bar{C}_{\frac{3}{2}}\times\bar{C}_{\frac{1}{2}i}$$

$$\bar{C}_{\frac{5}{2}i}=\bar{C}_{\frac{5}{2}}\times\bar{C}_{\frac{1}{2}i}$$

. . . .

$$\bar{C}_{(n+\frac{1}{2})i}=\bar{C}_{n+\frac{1}{2}}\times\bar{C}_{\frac{1}{2}i}$$

. . . .

$$\bar{C}_{\frac{1}{2}\bar{i}}=\{E, \bar{I}\}$$

$$\bar{C}_{\frac{3}{2}\bar{i}}=\bar{C}_{\frac{3}{2}}\times\bar{C}_{\frac{1}{2}\bar{i}}$$

$$\bar{C}_{\frac{5}{2}\bar{i}}=\bar{C}_{\frac{5}{2}}\times\bar{C}_{\frac{1}{2}\bar{i}}$$

. . . .

$$\bar{C}_{(n+\frac{1}{2})\bar{i}}=\bar{C}_{n+\frac{1}{2}}\times\bar{C}_{\frac{1}{2}\bar{i}}.$$

. . . .

Proof. It is very easy to verify that all the listed sets form groups. We shall prove now that the above list of non-evident subgroups is complete. Two cases have to be considered: (1) the subgroups with one odd-order symmetry axis, (2) the subgroups with several odd-order symmetry axes.

At the beginning the subgroups with one odd-order symmetry axis are taken into account. In this case every non-evident subgroup is a combination of the element listed in Theorem 2. Of course, not all possible combinations are allowed. One excludes the combinations leading to $\bar{E}$, because such combinations correspond to the evident groups. For example, $\{I, \bar{I}\}$ is excluded because $I\bar{I}=\bar{E}$. One can verify by inspection that the list of subgroups considered with one odd-order axis is complete.

Finally one should remark that the non-evident subgroup cannot contain two or more (case 2) nonparallel odd-order symmetry axes. It is well known that the point group (single or double) with more than one odd-order symmetry axis always contains at least one even-order axis, but such an axis cannot exist in the non-evident subgroups (Theorems 1 and 2).

These three theorems permit the subgroups of the double point group to be found, similarly as the Opechowski rules permit the classes of the double group to be found (*e.g.* Opechowski, 1940; Bradley & Cracknell, 1972; Backhouse, 1973, 1975).

From the geometrical point of view all the groups found in Theorem 3 are new. But, taking into account their abstract definitions, we should remark that they are isomorphic to the groups already known. For example, the group $\bar{C}_{\frac{3}{2}}$ is isomorphic to the group C_3, the group $\bar{C}_{\frac{1}{2}i}$ is isomorphic to the groups C_2, C_s, C_i, and so on.

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References

BACKHOUSE, N. B. (1973). *Physica*, **70**, 505–519.
BACKHOUSE, N. B. (1975). *J. Math. Phys. (NY)*, **16**, 443–447.
BRADLEY, C. J. & CRACKNELL, A. P. (1972). *The Mathematical Theory of Symmetry in Solids*. London: Clarendon Press.
GORZKOWSKI, W. (1976). *The Transitive Representations of the Crystallographic Point Groups* (in Polish). Thesis, Polish Academy of Sciences, Warsaw.
GORZKOWSKI, W. & SUFFCZYNSKI, M. (1978). *Bull. Acad. Pol. Sci. Cl.* 3, **26**, 563–566.
HALL, M. (1959). *The Theory of Groups*. New York: Macmillan.
OPECHOWSKI, W. (1940). *Physica*, **7**, 552–562.

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The New Double Space Groups

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Abstract

The definition of the double space groups is extended. All the new double space groups are classified.

The symmetry operations forming the space group G obey the following multiplication rule:

$$\{R_2|\mathbf{v}_2\}\{R_1|\mathbf{v}_1\}=\{R_2R_1|\mathbf{v}_2+R_2\mathbf{v}_1\}.$$

The space group G can be expressed as the sum of the left cosets of the translation group of one of the Bravais lattices T:

$$G=\{R_1|\mathbf{v}_1\}T+\{R_2|\mathbf{v}_2\}T+\cdots+\{R_h|\mathbf{v}_h\}T,$$

where the rotational parts $R_1, R_2, \ldots, R_h$ form one of the 32 crystallographic point groups.

In the case of double groups, for every element R_i of the single point group there are two corresponding elements: R_i and $\bar{R}_i$. We assume that both elements R_i and $\bar{R}_i$ have the same effect in acting on vectors $\mathbf{v}_j$:

$$\bar{R}_i\mathbf{v}_j=R_i\mathbf{v}_j.$$

The elements R_i and $\bar{R}_i$ obey the multiplication rule of the double point group.

The commonly used (*e.g.* Bradley & Cracknell, 1972) definition of the double space group G^+ corresponding to the single space group G is given by the formula:

$$G^+=\{R_1|\mathbf{v}_1\}T+\{\bar{R}_1|\mathbf{v}_1\}T+\{R_2|\mathbf{v}_2\}T+\{\bar{R}_2|\mathbf{v}_2\}T+\cdots+\{R_h|\mathbf{v}_h\}T+\{\bar{R}_h|\mathbf{v}_h\}T,$$

where R_i and $\bar{R}_i$ are the elements of the double point group corresponding to the operation R_i in the single point group formed by $R_1, R_2, \ldots, R_h$. The multiplication rules for the members of the double space group G^+ have the form:

$$\{R_2|\mathbf{v}_2\}\{R_1|\mathbf{v}_1\}=\{R_2R_1|\mathbf{v}_2+R_2\mathbf{v}_1\}$$
$$\{\bar{R}_2|\mathbf{v}_2\}\{R_1|\mathbf{v}_1\}=\{\bar{R}_2R_1|\mathbf{v}_2+R_2\mathbf{v}_1\}$$
$$\{R_2|\mathbf{v}_2\}\{\bar{R}_1|\mathbf{v}_1\}=\{R_2\bar{R}_1|\mathbf{v}_2+R_2\mathbf{v}_1\}$$
$$\{\bar{R}_2|\mathbf{v}_2\}\{\bar{R}_1|\mathbf{v}_1\}=\{\bar{R}_2\bar{R}_1|\mathbf{v}_2+R_2\mathbf{v}_1\}.$$

According to the definition we have 230 double space groups (as in the case of the single space groups). Each of these groups contains the pairs of elements: $\{R_i|\mathbf{v}_i\}$ and $\{\bar{R}_i|\mathbf{v}_i\}$.

It seems that the above definition is not complete. For example, the subgroup G_1^+ of the group G^+ formed by the elements

$$\{E|0\}T,$$

where T is the translational group and E denotes the identity, is not the double space group in the sense of the definition given above. This is a rather trivial example. However, the following example is not so trivial.

It is easy to verify that the set G_2^+ given by the formula:

$$G_2^+=\{E|0\}T+\{\overline{C_3^-}|0\}T+\{\overline{C_3^+}|0\}T,$$

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