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ERROR CORRECTIONS CORRECTED: A REMARK ON BERTAUT'S ARTICLE

« SIMPLE DERIVATION OF MAGNETIC SPACE GROUPS »

By

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ABSTRACT

According to Bertaut (1975), there is a number of incorrect assignments of symbols to orthorhombic magnetic space groups in the list published by Opechowski and Guccione (1965). We have checked all these symbol assignments. Contrary to Bertaut's assertion, there are no errors in the list of the OG (Opechowski-Guccione) symbols. On the other hand, there are errors in the list of the corresponding BNS (Belov-Neronova-Smirnova) symbols, although we do not always agree with the corrections indicated by Bertaut. Table I gives the corrected BNS symbols. In the Appendix, we illustrate by an example how the assigning of the OG and BNS symbols was done, and we formulate a conjecture as to the reason of the continuing disagreement between Bertaut and ourselves.

RÉSUMÉ

Corrections corrigées : remarque sur le mémoire de Bertaut « Dérivation simple de groupes d'espace magnétiques »

Selon Bertaut (1975), Opechowski et Guccione (1965), dans leur liste des groupes d'espace magnétiques, ont noté incorrectement certains groupes orthorhombiques. Nous avons examiné les symboles incriminés. Contrairement à ce qu'affirme Bertaut, les symboles OG (Opechowski-Guccione) sont tous corrects; en revanche, les symboles BNS (Belov-Neronova-Smirnova) ne le sont pas tous, mais nous ne sommes pas d'accord avec la plupart des corrections indiquées par Bertaut. Le tableau I donne les symboles BNS corrigés. Dans l'Appendice, nous illustrons d'un exemple la méthode employée pour obtenir les symboles OG et BNS et nous formulons une hypothèse concernant la raison du désaccord persistant entre Bertaut et nous-mêmes.

In a recent paper, Bertaut [1] reports a number of alleged errors in the list of the 1421 classes of equivalent magnetic space groups given by Opechowski and Guccione [2]. In that list to each class two symbols are assigned: one symbol specifies the class in a way adapted to the derivation of all these classes by the method of Opechowski and Guccione, the other symbol is that introduced earlier by Belov, Neronova and Smirnova [3]. We shall refer to these two kinds of symbols as « OG symbols » and « BNS symbols ». The alleged errors are correspondingly of two kinds:

1) alleged errors in the list of all classes of magnetic space groups (m. s. g.) specified by means of OG symbols;

2) alleged errors in pairing an OG symbol and a BNS symbol which specify the same class of m. s. g.

With regard to 1), Bertaut considers only that part of the Opechowski-Guccione list which contains the m. s. g. that belong to the families of space groups whose point group is *mmm* and whose lattice is either C or I, thus 58 classes of m. s. g. altogether. He claims that some of the classes of m. s. g. occur in the Opechowski-Guccione list twice and some not at all. We have examined these alleged errors and we have found that the allegations are incorrect in all cases. In other words, each of the 58 OG symbols in the Opechowski-Guccione list corresponds to a different class of m. s. g., and no symbol of any class is missing (there is, however, one misprint, reprinted by Bertaut without change: the symbol $C_I m'm'a'$ should read $C_I m'ma'$ or $C_I m'ma$, the two latter symbols specifying the same class of m. s. g.).

With regard to 2), here Bertaut considers the same 58 classes of m. s. g., and points out that on several occasions Opechowski and Guccione have paired the same BNS symbol with different OG symbols, which evidently means that there are some errors in the pairing. We have reexamined the pairing of the BNS symbols with the OG symbols in all 58 cases and we have found that in all those cases in which the pairing is incorrect the appropriate BNS symbol differs from the inappropriate listed one only in the subscript attached to the capital letter (P or I) denoting the type of lattice. This is not accidental. It must be realized that the OG symbol specifies a class of m. s. g. belonging to the family of a space group F by indicating the subgroup D of index 2 in F which consists of all those elements of F that are not combined with time inversion. To obtain the BNS symbol of a m. s. g. from the OG symbol, one has to replace the OG symbol by the standard international symbol of D, and then attach an appropriate subscript to it. Thus, the standard international symbol of D is given correctly by Opechowski and Guccione for all 58 cases, and the errors crept only in when rewriting the standard international symbol of D as the BNS symbol for the corresponding m. s. g. We list in Table I all those entries in the Opechowski-Guccione list where the subscript in the BNS symbol had to be replaced by the correct one: in the first column from the left we list the OG symbols as they appear in the original Opechowski-Guccione list, and in the second column the appropriate BNS symbols. We should mention that Bertaut, in his Tables IV, V and VI, replaces in a number of cases (other than those listed in our Table I) a BNS symbol given correctly by Opechowski and Guccione by an inappropriate one.

In an Appendix, here below, we restate much more in detail than in Opechowski and Guccione [2] the conventions on which the assignment of the OG symbol to a m. s. g. of the kind M_R is based. All the 58 classes of m. s. g. considered by Bertaut are classes of m. s. g. of the kind M_R (In the terminology of Opechowski and Guccione [2], each m. s. g. is either of the kind M_R or M_T). Furthermore, we illustrate, by an example in the Appendix, how actually the assigning of an OG symbol to a m. s. g. is done (and also of the correspondings BNS symbol); and how the equivalence, or inequivalence, of m. s. g. is established.

TABLE I

$C_P mc'm$	$P_A mmn$	$C_P m'mm$	$P_B mma$
$C_P mcm'$	$P_A nma$	$C_P mm'm'$	$P_B mna$
$C_P m'c'm$	$P_B nma$	$C_I m'mm$	$I_a mma$
$C_P mc'm'$	$P_A nnm$		
$C_P m'c'm'$	$P_B nna$	$C_P c'cm$	$P_A mna$
		$C_P cc'm'$	$P_A nna$
$C_P mca$	$P_A bam$		
$C_P m'ca$	$P_A cca$	$C_P mma$	$P_A ccm$
$C_P mca'$	$P_B bcm$	$C_P m'ma$	$P_B cca$
$C_P m'c'a$	$P_a ccn$	$C_P mma'$	$P_A bcm$
$C_P m'c'a'$	$P_A bcn$	$C_I mma$	$I_a bam$
		$C_P cca$	$P_A ban$
		$C_P cca'$	$P_B bcn$

* * *

APPENDIX

In order to obtain an OG symbol for a magnetic space group of the kind M_R, one has to follow a sequence of steps described below.

I. In the case of a space group belonging to Class *f* (*f* = 1, 2, 3... 230), the number *f* being that assigned to that class in ITXC (= International Tables for X-Ray Crystallography), we find in ITXC, a specification of the coordinate system used, and, in terms of that coordinate system, a specification of the lattice (= subgroup of translations) T of one space group F belonging to class *f*, and also indirectly a specification of a set of *n* coset representatives of T in F, where *n* is the index of T in F. « Indirectly », because what is actually specified are the coordinates of *n* (or a small multiple of *n*) equivalent positions; among these there are exactly *n* positions for which a list of coordinates is printed. That list then uniquely determines a set of coset representatives of T in F, and the set so determined will be called in what follows « the standard set of coset representatives of T in F »; see *Example* below. « The standard international symbol » of class *f* of space groups printed at the top of the corresponding page of ITXC is supposed to specify T and to indicate a set of coset representatives of T in F, but the set so indicated is, unfortunately, in some cases different from the standard set just defined. To avoid this ambiguity we have adopted the following convention (the same convention was adopted by Opechowski and Guccione when preparing their list of the magnetic space groups) : we always use the standard international symbol printed at the top of a page of ITXC to denote class f to which that space group F belongs which is defined by the lattice T specified on that page and by the standard set of coset representatives of T in F specified on the same page; « always », that is, even if the standard international symbol of F would indicate a choice of a set of coset representatives of T in F which is different from the standard set.

Alternatively, one could avoid the ambiguity by using the fact that a set of coset representatives of T in F can be chosen in an infinity of ways, and, if necessary, choosing, instead of the standard set, a set which is not in disagreement with the indications of the standard international symbol of F. While our convention makes it possible to use ITXC as they are, and that is why it was adopted, this alternative way of avoiding the ambiguity is tantamount, for each class f for which such an ambiguity occurs, to a modification of the text of the corresponding page of ITXC: one has to replace the set of coordinates of n equivalent positions as printed by a new set which determines the chosen set of coset representatives. In other words, this alternative way consists in adopting the convention of not using the text of ITXC as it is, for each such class f, but modifying it appropriately.

At this point it is important to realize that the same OG symbol (and, consequently, the corresponding BNS symbol) may denote two different classes of magnetic space groups according as one adopts our convention or the alternative one.

This dependence of the meaning of an OG symbol on the convention adopted is the origin of the disagreement between Prof. Bertaut and us. Prof. Bertaut does not like our convention and gives preference to the convention implied by the second alternative, which is of course his good right to do. But, when he sets out to decide about correctness or incorrectness of the assignments of the OG symbols made on the basis of our convention, and in doing so ignores the latter, he is bound to make statements which will often be, from the point of view of anyone who accepts our convention, nothing more than incorrect allegations of error; and this is precisely what has happened. Prof. Bertaut apparently believes that our convention is not self-consistent (otherwise he would not speak of our « falling into a trap » nor would he call a standard set of coset representative « non adequate » whenever it is different from that chosen on the basis of his convention); if so, we regret that we have not been able to convince him that he is mistaken.

II. EXAMPLE Class 67 (*Cmma*, p. 156 of ITCX). Lattice:

$$C = \left\langle \left(1 \mid \tfrac{1}{2}\tfrac{1}{2}0\right), \left(1 \mid \tfrac{1}{2}\tfrac{\bar{1}}{2}0\right), (1 \mid 0\,0\,1) \right\rangle.$$

Coordinates of equivalent positions (printed on that page):

$$x, y, z\,;\; x, \bar{y}, \bar{z}\,;\; \tfrac{1}{2} - x, y, \bar{z}\,;\; \tfrac{1}{2} - x, \bar{y}, z\,;$$
$$\bar{x}, \bar{y}, \bar{z}\,;\; \bar{x}, y, z\,;\; \tfrac{1}{2} + x, \bar{y}, z\,;\; \tfrac{1}{2} + x, y, \bar{z}.$$

Standard set of coset representatives of C in *Cmma*:

$$(1)\quad \left\{ \begin{aligned} &(1 \mid 0\,0\,0), (2_x \mid 0\,0\,0), \left(2_y \mid \tfrac{1}{2}0\,0\right), \left(2_z \mid \tfrac{1}{2}0\,0\right), \\ &(\bar{1} \mid 0\,0\,0), (m_x \mid 0\,0\,0), \left(m_y \mid \tfrac{1}{2}0\,0\right), \left(m_z \mid \tfrac{1}{2}0\,0\right) \end{aligned} \right\}$$

III. Next we select one of the subgroups of index 2 of the lattice T of the space group F considered in (II), in what follows called a *sublattice* T^D of T (and also of F) and we specify that sublattice by means of its three generators, using the same coordinate system as that used in (II) and we also specify one translation, to be denoted by $t_\alpha = (1 \mid u_\alpha v_\alpha w_\alpha)$ which belongs to T but not to T^D. Then $T = T^D + t_\alpha T^D$. Each subgroup D_R of index 2 of F, which has as a lattice the sublattice T^D, can then be specified by a set of coset representatives of T^D in D_R, which is obtained from the standard set of coset representatives of T in F by multiplying by t_α some (or possibly none) of these coset representatives. *N. B.* The converse is not true: by multiplying by t_α some of the coset representatives in the standard set one does not necessarily obtain a set of coset representatives of T^D in some proper subgroup of F.

Each such subgroup D_R of F is assigned a OG symbol as follows: (*a*) the lattice symbol T in the standard international symbol of F is replaced by the symbol of the lattice T^D of D_R; (*b*) if a coset representative (of T in F) whose rotational part is 2_j or m_j ($j = x, y, z$) has been multiplied by t_α, then a dash is attached to the integer, 2, or letter, m, a, b, c, d, n, which occupies the j-th location in the standard international symbol of F (the rule (*b*) is here formulated for the orthorhombic system).

EXAMPLE *(continued)*. If we select as the sublattice T^D of C the group of translations

$$C_I = \left\langle \left(1 \mid \tfrac{1}{2}\tfrac{1}{2}1\right), (1 \mid 0\,1\,0), (1 \mid 1\,0\,0) \right\rangle$$

and $t_\alpha = \left(1 \mid \tfrac{1}{2}\tfrac{1}{2}0\right)$ then $C = C_I + \left(1 \mid \tfrac{1}{2}\tfrac{1}{2}0\right)C_I$. One of the subgroups D_R of *Cmma* is the subgroup whose lattice is C_I and such that the coset representatives of C_I in D_R are those constituting the set (1); the OG symbol of that subgroup D_R is thus C_Imma. Another subgroup D_R of *Cmma* with lattice C_I is the space group such that the set of coset representatives of C_I in D_R is that obtained from the set (1) by multiplying the representatives in the second row by $t_\alpha = \left(1 \mid \frac{1}{2}\frac{1}{2}0\right)$ on the left; the OG symbol for this subgroup D_R is thus $C_Im'm'a'$. In fact, a complete list of the subgroups D_R with the lattice C_I consists of 8 subgroups D_R of *Cmma* as follows:

$$
\begin{array}{lllll}
 & C_Imma & C_Im'm'a' & C_Imma' & C_Im'm'a \\
(2) & C_Im'ma & C_Im'ma' & & \\
 & C_Imm'a & C_Imm'a' & &
\end{array}
$$

IV. A magnetic space group M_R that belongs to the family of a space group F has always the form

$$M_R = D_R + (F - D_R)E',$$

where E′ is time inversion. Therefore M_R is uniquely specified by specifying F and D_R. Since the OG symbol of D_R as described in (III) specifies both D_R and F, it can be used, and is used also as a symbol of the corresponding magnetic space group M_R, and also as a symbol of the class of magnetic space groups to which that M_R belongs. *N. B.* If two subgroups D_R of F which have a common lattice belong to the same class of space groups, then the two corresponding magnetic space groups M_R belong to the same class of magnetic space groups. It follows that two different OG symbols (differing from each other by the number and location of dashes) may denote the same class of magnetic space groups. As a rule, O. and G. have used the OG symbol with the smallest number fo dashes.

EXAMPLE *(continued)*. The symbols in the top line of (2), as symbols of magnetic space groups, specify the space group F = *Cmma* and the subgroups $D_R = C_Imma$ or $C_Im'm'a'$ or C_Imma' or $C_Im'm'a$. They have been written out in the same line because they turn out to belong to the same class of magnetic space groups, which is denoted by C_Imma. Similarly, the symbols in the second line of (2), as symbols of magnetic space groups, denote two magnetic space groups belonging to the class $C_Im'ma$. Finally, the symbols in the third line (2) denote two magnetic space groups belonging to the class $C_Imm'a$.

V. A subgroup D_R (to which we have assigned a OG symbol as explained in (III)) of F is a space group, and as such can be assigned a standard international symbol. To find that symbol, we subject the lattice T^D of D_R, and the set of coset representatives of T^D in D_R to a similarity transformation such that, as a result of it, T^D and the set of coset representatives become identical with a lattice and a standard set of coset representatives of a class of space groups. If this class is class *f*, then the standard international symbol of D_R will be that of class *f*. *N. B.* It is this standard international symbol of D_R, with an appropriate subscript attached to the symbol of the lattice, which serves in the BNS notation as a symbol of that class of magnetic space groups which, in the OG notation, is denoted by the OG symbol of D_R. The « appropriate subscript » indicates, in a notation explained by B., N. and S., what we have here denoted by t_α.

EXAMPLE *(continued)*. We show that the space group $C_Im'ma = C_I\, 2/m'\, 2'/m\, 2'/a$ belongs to Class 73, whose standard international symbol is *Ibca*. First, we change the unit length along the *z*-axis so as to obtain:

$$C_I = \left\langle \left(1 \mid \tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\right), (1 \mid 0\,1\,0)\ (1 \mid 1\,0\,0) \right\rangle.$$

Next, from (1) and from the meaning of the dashes (explained in (III), rule (*b*)) in the symbol $C_I\, 2/m'\, 2'/m\, 2'/a$, it follows that the coset representatives of C_I in $C_Im'ma$ are:

$$\Big\{(1 \mid 0\,0\,0),\ (2_x \mid 0\,0\,0),\ \left(2_y \mid 0\tfrac{1}{2}0\right),\ \left(2_z \mid 0\tfrac{1}{2}0\right),$$
$$\left(\bar{1} \mid \tfrac{1}{2}\tfrac{1}{2}0\right),\ \left(m_x \mid \tfrac{1}{2}\tfrac{1}{2}0\right),\ \left(m_y \mid \tfrac{1}{2}0\,0\right),\ \left(m_z \mid \tfrac{1}{2}0\,0\right)\Big\}$$

Shifting the origin of the coordinate system by means of the translation $\left(1 \mid \frac{1}{4}\frac{1}{4}0\right)$ we obtain:

$$\Big\{(1 \mid 0\,0\,0),\ \left(2_x \mid 0\tfrac{1}{2}0\right),\ \left(2_y \mid \tfrac{1}{2}\tfrac{1}{2}0\right),\ \left(2_z \mid \tfrac{1}{2}0\,0\right)$$
$$(\bar{1} \mid 0\,0\,0),\ \left(m_x \mid 0\tfrac{1}{2}0\right),\ \left(m_y \mid \tfrac{1}{2}\tfrac{1}{2}0\right),\ \left(m_z \mid \tfrac{1}{2}0\,0\right)\Big\}$$

Substituting *y* for *x*, and $\bar{x}$ for *y*, we transform this set into the set:

$$\Big\{(1 \mid 0\,0\,0),\ \left(2_x \mid \tfrac{\bar{1}}{2}\tfrac{1}{2}0\right),\ \left(2_y \mid \tfrac{\bar{1}}{2}0\,0\right),\ \left(2_z \mid 0\tfrac{1}{2}0\right)$$
$$(\bar{1} \mid 0\,0\,0),\ \left(m_x \mid \tfrac{\bar{1}}{2}\tfrac{1}{2}0\right),\ \left(m_y \mid \tfrac{\bar{1}}{2}0\,0\right),\ \left(m_z \mid 0\tfrac{1}{2}0\right)\Big\}$$

Finally, multiplying on the left the 2nd and the 6th coset representative in the latter set by the translation $\left(1 \mid \frac{1}{2}\frac{\bar{1}}{2}\frac{1}{2}\right)$, and the 3rd and the 7th by $(1 \mid 1\,0\,0)$, both translations belonging to C_I, we obtain:

$$\Big\{(1 \mid 0\,0\,0),\ \left(2_x \mid 0\,0\tfrac{1}{2}\right),\ \left(2_y \mid \tfrac{1}{2}0\,0\right),\ \left(2_z \mid 0\tfrac{1}{2}0\right),$$
$$(\bar{1} \mid 0\,0\,0),\ \left(m_x \mid 0\,0\tfrac{1}{2}\right),\ \left(m_y \mid \tfrac{1}{2}0\,0\right),\ \left(m_z \mid 0\tfrac{1}{2}0\right)\Big\}$$

This is the standard set of coset representatives of the lattice I in the space group belonging to Class 73, I*bca*, see p. 165 of ITXC. The translation $t_\alpha = \left(1 \mid \frac{1}{2}\frac{1}{2}0\right)$ becomes, after the substitution just made,

$$\left(1 \mid \frac{\bar{1}}{2}\frac{1}{2}0\right) = \left(1 \mid \frac{1}{2}\frac{1}{2}0\right) = \left(1 \mid 0\,0\,\frac{1}{2}\right), \bmod C_I ;$$

therefore the BNS symbol for the magnetic space group $C_I m'ma$ becomes $I_c bca$.

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