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# Opechowski–Guccione-like symbols labelling magnetic space groups independent of tabulated (0, 0, 0)+ sets

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For the magnetic space-group types with a black and white lattice two sets of symbols have been proposed: the BNS symbols [Belov *et al.* (1957). *Sov. Phys. Crystallogr.* **2**, 311–322] and the OG symbols [Opechowski & Guccione (1965). *Magnetism*, edited by G. T. Rado & H. Suhl, Vol. II, Part A, pp. 105–165. New York: Academic Press]. Whereas generators of the group can be read off the BNS symbol, *International Tables for X-ray Crystallography* (1952) must be consulted to interpret the OG symbols. In the cases where the black and white lattice is centred, it is shown how the OG symbols can be modified so that generators of the group can be deduced directly from the symbol.

## 1. Introduction

Considering as possible symmetry operations of crystals the isometries of three-dimensional space, *i.e.* translations, rotations, 'space inversion' $\bar{1}$ and their combinations, the 230 types of ordinary space groups are obtained. Admitting also 'time inversion' $1'$ (which inverts the spin direction) and its combination with isometries, we obtain the 1651 Shubnikov space-group types. Let **G** be an ordinary space group and **H** a subgroup of index 2. Among the 1651 types there are 230 of the form **G**, 230 of the form $\mathbf{G} + \mathbf{G}1'$ and 1191 of the form $\mathbf{H} + (\mathbf{G} - \mathbf{H})1'$. **H** is an isotranslational subgroup for 674 among the 1191 types, and an isoclass subgroup for the remaining 517 types. In the language of two-colour groups, where $1'$ is interpreted as exchanging black and white (or black and red for typographical reasons), we speak of 230 monochrome types, 230 grey types, 674 black–white types of the first kind (BW1 types) and 517 black–white types of the second kind (BW2 types).

Using simple rules, a set of generators of an ordinary space group can be read off its Hermann–Mauguin symbol (HMS) (Hermann, 1928, 1931; Mauguin, 1931; Burzlaff & Zimmermann, 1983). Symbols for the 1651 Shubnikov space-group types based on the HMS, called BNS symbols, were first introduced by Belov *et al.* (1957*a*,*b*). For the black–white group $\mathbf{H} + (\mathbf{G} - \mathbf{H})1'$ of the first kind the BNS symbol differs from the HMS for **G** in that the symbols for (screw) rotations and (glide) reflections belonging to $\mathbf{G} - \mathbf{H}$ are primed. A primed symbol means that the corresponding generator is combined with $1'$.

The 517 BW2 types can be written as $\mathbf{H} + \mathbf{H}\mathbf{t}1'$, where **t** is a translation not contained in **H** but such that 2**t** lies in **H**. The BNS symbol of these groups is based on the HMS of the monochrome subgroup **H** by adding a subscript to the first letter of the HMS of **H**: the subscripts *a*, *b*, *c* mean that $\mathbf{t} = \mathbf{a}/2$, $\mathbf{b}/2$, $\mathbf{c}/2$; similarly *A*, *B*, *C* mean that $\mathbf{t} = (\mathbf{b} + \mathbf{c})/2$, $(\mathbf{c} + \mathbf{a})/2$, $(\mathbf{a} + \mathbf{b})/2$; *I* means $\mathbf{t} = (\mathbf{a} + \mathbf{b} + \mathbf{c})/2$; and *s* means that **t** may be chosen as $\mathbf{a}/2$, $\mathbf{b}/2$ or $\mathbf{c}/2$. The BW2 groups are generated by $\boldsymbol{t}1'$ and a set of generators for **H**.

Finally, the BNS symbol of the grey group $\mathbf{G} + \mathbf{G}1'$ is obtained by placing $1'$ after the HMS of **G**. The grey groups are generated by $1'$ and a set of generators for **G**.

We conclude that a set of generators for the group can be read off its HMS or BNS symbol without the need to consult a space-group table. This is in marked contrast to the Schoenflies symbols for the ordinary (*i.e.* monochrome) space-group types, from which only the crystal class can be read off immediately whereas a table of the 230 space-group types has to be consulted for further information on the type.

The monochrome, the grey and all the black–white types based on the same HMS form a BNS superfamily. Whereas the BNS symbols of monochrome, grey and BW1 groups have become generally recognized standards, Opechowski & Guccione (1965) proposed different symbols for the 517 BW2 types, the OG symbols, based on the HMS of **G**, not of **H** in the decomposition $\mathbf{H} + (\mathbf{G} - \mathbf{H})1'$. The monochrome, the grey and all the black–white types based on the same HMS form an OG superfamily. Obviously, there are 230 BNS superfamilies and 230 OG superfamilies; the classification into BNS and OG superfamilies coincides for monochrome, grey and BW1 types but differs for BW2 types.

With six exceptions, the symbols proposed by Opechowski & Guccione (1965) are obtained by adding a subscript to the first letter of the HMS of **G**, and, possibly, adding primes to the symbols for (screw) rotations and (glide) reflections.[1] The subscript indicates the sublattice defined by the unprimed translations. The volume $V_{\mathbf{H}}$ of the conventional cell of **H** may be larger than the volume $V_{\mathbf{G}}$ of the conventional cell of **G**, $V_{\mathbf{H}} = 2^n V_{\mathbf{G}}$, where $n = 0, 1, 2$ or 3. Whereas the conventional cell of **H** is spanned by three unprimed translations, the conventional cell of **G** will be spanned by $n$ primed and $3 - n$ unprimed translations. The 22 types of black–white lattices are illustrated and the corresponding OG and BNS symbols given in many publications, see *e.g.* Figs. 1.5.2.1 to 1.5.2.7 in Borovik-Romanov & Grimmer (2003). They are summarized in Table 1 together with the corresponding values of $n$.

Unfortunately, at least three different interpretations of the OG symbols of BW2 groups have been proposed, making the correspondence between BNS and OG symbols not unique in several cases. The ambiguities in interpreting OG symbols are in marked contrast to the case of BNS symbols, where the unprimed symmetry operations coincide with the symmetry operations of the ordinary space group in the BNS superfamily and the primed symmetry operations are simply obtained by combining the unprimed symmetry operations with the primed translation specified by the subscript in the BNS symbol. OG symbols for the 517 BW2 types were first published by Opechowski & Guccione (1965) as Table III together with the corresponding BNS symbol. Bertaut (1975) gave a list of the cases in class *mmm* where his interpretation of OG symbols deviated from theirs. Opechowski & Litvin (1977) agreed that for 21 OG symbols the BNS equivalents given in Table III of Opechowski & Guccione (1965) were wrong, but they denied that the list of OG symbols in Table III contained errors.[2] In an appendix, Opechowski & Litvin (1977) explained how the meaning of the OG symbols depends, in the cases where the conventional cell of **G** is centred, on the (0, 0, 0)+ set of positions selected in Volume I of *International Tables for X-ray Crystallography* (1952), which will be referred to as ITXC52. Bertaut (1977) replied that the Opechowski–Litvin convention leads to inconsistences with ITXC52 for the superfamilies *Cmca*, *Cmma* and *Ccca*. In Volume A of *International Tables for Crystallography* (1983), which will be referred to as ITC83, a different (0, 0, 0)+ set was selected in some cases, which prompted Litvin (1998) to propose interpreting the OG symbols on the choice made in ITC83. This change led to new standard OG symbols for 29 types; in many of these cases the new standard symbol has exactly the same form as an old one, but the types denoted by the two symbols are interchanged. The situation is illustrated in Fig. 1 with an example from superfamily 67: *Cmma*.

As generators for the group shown in this figure we may choose the translation **a** downwards, **b** to the right, **c** perpendicular to the plane of the figure, the primed translation $\frac{1}{2}(\mathbf{a}' + \mathbf{b}')$, the mirror reflections $m\ \ 0, y, z$ and $m\ \ x, 0, z$, and the glide reflection $a\ \ x, y, 0$. [The origin of the coordinate system then lies at the intersection of the three (glide) mirror planes.] These generators are suggested by the BNS symbol and by the OG symbol proposed by Bertaut (1975). Just looking at the OG symbol proposed by Opechowski & Guccione (1965) we would expect a primed mirror plane perpendicular to the **b** direction, which is not there. Similarly, looking at the OG symbol proposed by Litvin (1998) we would expect a glide mirror $a'$ in the plane of the figure, instead we have glide mirrors $a$ and $b'$. I guess that this is what Bertaut (1977) meant by 'inconsistencies with ITXC52'. I want to stress that it does not mean that the conventions of Opechowski & Guccione (1965) or of Litvin (1998) are not self-consistent; they just lead to symbols from which we immediately can deduce only the

**Table 1**
OG and BNS symbols for the black–white lattice types.

| Bravais system | $n$ | OG symbol | BNS symbol |
|---|---|---|---|
| Anorthic | 1 | $aP_{2s} = aP_{2c}$ | $aP_s = aP_c$ |
| Monoclinic | 1 | $mP_{2a}$, $mP_{2c}$ | $mP_a$, $mP_c$ |
| | 1 | $mP_{2b}$ | $mP_b$ |
| | 2 | $mP_C$ | $mC_a$ |
| | 1 | $mC_{2c}$ | $mC_c$ |
| | 0 | $mC_P$ | $mP_C$, $mP_A$ |
| Orthorhombic | 1 | $oP_{2a}$, $oP_{2b}$, $oP_{2c}$ | $oP_a$, $oP_b$, $oP_c$ |
| | 2 | $oP_C$, $oP_A$ | $oC_a$, $oA_c$ |
| | 3 | $oP_F$ | $oF_s = oF_I$ |
| | 1 | $oC_{2c}$, $oA_{2a}$ | $oC_c$, $oA_a$ |
| | 0 | $oC_P$, $oA_P$ | $oP_C$, $oP_A$ |
| | 1 | $oC_I$, $oA_I$ | $oI_c$, $oI_a$ |
| | 0 | $oF_C$, $oF_A$ | $oC_A$, $oA_C$ |
| | 0 | $oI_P$ | $oP_I$ |
| Tetragonal | 1 | $tP_{2c}$ | $tP_c$ |
| | 1 | $tP_{a-b,a+b} = tP_P$ | $tP_C$ |
| | 2 | $tP_I$ | $tI_c$ |
| | 0 | $tI_P$ | $tP_I$ |
| Rhombohedral | 1 | $rR_{b+c,c+a,a+b} = rR_R$ | $rR_I$ |
| Hexagonal | 1 | $hP_{2c}$ | $hP_c$ |
| Cubic | 3 | $cP_F$ | $cF_s = cF_I$ |
| | 0 | $cI_P$ | $cP_I$ |

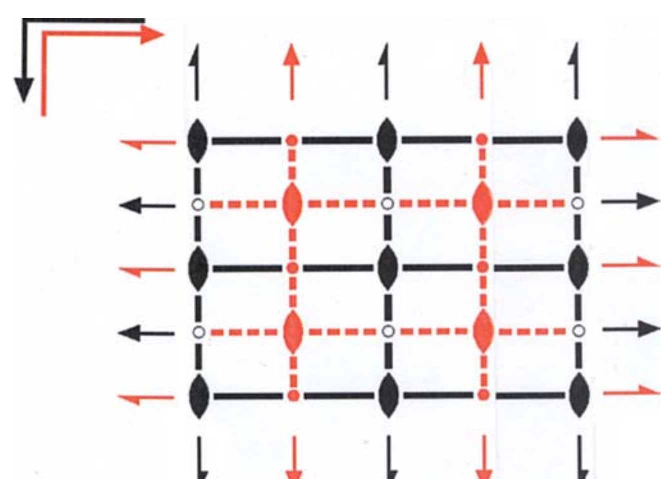

**Figure 1**
Symmetry diagram for the space group with BNS symbol $P_Cmma$. OG symbol according to Opechowski & Guccione (1965): $C_Pmm'a$, according to Litvin (1998): $C_Pmma'$. Symbol proposed by Bertaut (1975) and this paper: $C_Pmma$.

[1] The six exceptions concern the three trigonal enantiomorphic pairs, where Opechowski & Guccione (1965) used the HMS of the enantiomorphic partner ($P3_1 \leftrightarrow P3_2$, $P3_112 \leftrightarrow P3_212$, $P3_121 \leftrightarrow P3_221$) to construct the OG symbol.
[2] Four OG symbols were corrected later in a supplement to Litvin (2008): $P_{2b}c'ca \rightarrow P_{2b}c'ca'$, $P_P4_2'/m'mc \rightarrow P_P4_2'/m'mc'$, $P_{2c}6'22 \rightarrow P_{2c}6'22'$, $P_{2c}6_2'22 \rightarrow P_{2c}6_2'22'$.

**Table 2**
The 58 OG superfamilies with a centred conventional cell that contain BW2 types: the (0, 0, 0)+ sets corresponding to the proposed OG-like symbols, different choices in *International Tables*.

An asterisk (*) in column 4 indicates that the (0, 0, 0)+ set does not correspond to a group.

| 1<br>Number and name of the OG superfamily | 2<br>(0, 0, 0)+ set corresponding to the proposed interpretation | 3<br>(0, 0, 0)+ set in ITC83 if different from column 2 | 4<br>(0, 0, 0)+ set in ITXC52 if different from column 2 |
|---|---|---|---|
| 5: $C2$ | 3: $P2$ | | |
| 8: $Cm$ | 6: $Pm$ | | |
| 9: $Cc$ | 7: $Pc$ | | |
| 12: $C2/m$ | 10: $P2/m$ | | |
| 15: $C2/c$ | 13: $P2/c$ | | |
| 20: $C222_1$ | 17: $P222_1$ | | |
| 21: $C222$ | 16: $P222$ | | |
| 22: $F222$ | 16: $P222$ | | |
| 23: $I222$ | 16: $P222$ | | |
| 24: $I2_12_12_1$ | 19: $P2_12_12_1$ | | |
| 35: $Cmm2$ | 25: $Pmm2$ | | |
| 36: $Cmc2_1$ | 26: $Pmc2_1$ | | |
| 37: $Ccc2$ | 27: $Pcc2$ | | |
| 38: $Amm2$ | 25: $Pmm2$ | | |
| 39: $Abm2$ | 28: $Pbm2$ ($Pma2$) | | |
| 40: $Ama2$ | 28: $Pma2$ | | |
| 41: $Aba2$ | 32: $Pba2$ | | |
| 42: $Fmm2$ | 25: $Pmm2$ | | |
| 44: $Imm2$ | 25: $Pmm2$ | | |
| 45: $Iba2$ | 32: $Pba2$ | | 27: $Pcc2$ |
| 46: $Ima2$ | 28: $Pma2$ | | |
| 63: $Cmcm$ | 51: $Pmcm$ ($Pmma$) | | |
| 64: $Cmca$ | 57: $Pmca$ ($Pbcm$) | 55: $Pmcb$ ($Pbam$) | 55: $Pmcb$ ($Pbam$) |
| 65: $Cmmm$ | 47: $Pmmm$ | | |
| 66: $Cccm$ | 49: $Pccm$ | | |
| 67: $Cmma$ | 51: $Pmma$ | 51: $Pmmb$ ($Pmma$) | 49: $Pmaa$ ($Pccm$) |
| 68: $Ccca$ | 54: $Pcca$ | | 60: $Pcnb$ ($Pbcn$) |
| 69: $Fmmm$ | 47: $Pmmm$ | | |
| 71: $Immm$ | 47: $Pmmm$ | | |
| 72: $Ibam$ | 55: $Pbam$ | | 49: $Pccm$ |
| 73: $Ibca$ | 61: $Pbca$ | | (*) |
| 74: $Imma$ | 51: $Pmma$ | 51: $Pmmb$ ($Pmma$) | 51: $Pmmb$ ($Pmma$) |
| 79: $I4$ | 75: $P4$ | | |
| 80: $I4_1$ | 76: $P4_1$ | | (*) |
| 82: $I\bar{4}$ | 81: $P\bar{4}$ | | |
| 87: $I4/m$ | 83: $P4/m$ | | |
| 97: $I422$ | 89: $P422$ | | |
| 98: $I4_122$ | 91: $P4_122$ | | (*) |
| 107: $I4mm$ | 99: $P4mm$ | | |
| 108: $I4cm \Rightarrow I4cc$ | 103: $P4cc$ | | 100: $P4bm$ |
| 119: $I\bar{4}m2$ | 115: $P\bar{4}m2$ | | |
| 120: $I\bar{4}c2$ | 116: $P\bar{4}c2$ | | |
| 121: $I\bar{4}2m$ | 111: $P\bar{4}2m$ | | |
| 139: $I4/mmm$ | 123: $P4/mmm$ | | |
| 140: $I4/mcm \Rightarrow I4/mcc$ | 124: $P4/mcc$ | | |
| 146: $R3$ | 143: $P3$ | | |
| 148: $R\bar{3}$ | 147: $P\bar{3}$ | | |
| 155: $R32$ | 150: $P321$ | | |
| 160: $R3m$ | 156: $P3m1$ | | |
| 166: $R\bar{3}m$ | 164: $P\bar{3}m1$ | | |
| 197: $I23$ | 195: $P23$ | | |
| 199: $I2_13$ | 198: $P2_13$ | | |
| 204: $Im\bar{3}$ | 200: $Pm\bar{3}$ | | |
| 206: $Ia\bar{3}$ | 205: $Pa\bar{3}$ | | (*) |
| 211: $I432$ | 207: $P432$ | | |
| 214: $I4_132$ | 213: $P4_132$ | | 212: $P4_332$ |
| 217: $I\bar{4}3m$ | 215: $P\bar{4}3m$ | | |
| 229: $Im\bar{3}m$ | 221: $Pm\bar{3}m$ | | |

affine OG superfamily to which the type belongs, not the type itself. Combining a left-handed and the corresponding right-handed 'crystallographic' OG superfamily (*e.g.* $P3_1 \leftrightarrow P3_2$) into an 'affine' OG superfamily, 219 'affine' OG superfamilies are obtained. That only the affine not the crystallographic OG superfamily can be read off the OG symbol is due to the six trigonal exceptions mentioned earlier. To find the type, one has to consult ITXC52 or ITC83, respectively, and to follow the procedure described in Opechowski & Litvin (1977). If the (0, 0, 0)+ sets given in ITC83 are used, then all the symmetry operations that correspond to an element in the (0, 0, 0)+ set are unprimed if the OG symbol contains no primes. This is no longer true in general if the (0, 0, 0)+ sets given in ITXC52 are used, because those (0, 0, 0)+ sets do not always correspond to a subgroup of the group under consideration, as indicated in Table 2. Litvin (2001) nevertheless proposed returning to the conventions based on ITXC52, considering that possible further changes of the (0, 0, 0)+ set in future editions of the *International Tables* would add to the confusion. Because consulting ITXC52 and applying the procedure described in Opechowski & Litvin (1977) in order to interpret the OG symbols is rather cumbersome, Litvin (2008) prepared tables that describe (among others) the BW2 types defined by the conventions of Opechowski & Guccione (1965), in a similar way as the ordinary space-group types are described in ITC83. The situation is then similar to the case of Schoenflies symbols, for which tables also have to be consulted to find the type designated by the symbol.

Notice that the choice of the (0, 0, 0)+ set affects the type denoted by an OG symbol only if the conventional cell of **G** is centred, *i.e.* if the first letter of the OG symbol is not *P*. We shall first deal with these cases, which comprise 230 among the 517 BW2 types.

Erroneously thinking that the OG symbols of BW2 types given by Opechowski & Guccione (1965) or by Litvin (1998) contain generating (screw) reflections and (glide) planes similar to the symbols of BW1 types, one nevertheless obtains the correct result for 181 among the 230 types in the first case and for 199 types in the second case, whereas the symbols proposed by Bertaut (1975) give the correct result for all 70 types in crystal class *mmm*. In §2 it will be shown how OG-like symbols for the 230 types can be defined that can be interpreted without the help of tables, similar to the BNS symbols.

ITC83 also explicitly gives for the (0, 0, 0)+ set of general positions the corresponding set of symmetry operations mapping position *x*, *y*, *z* into the positions in the (0, 0, 0)+ set. For a space group **G** with a centred conventional cell possessing isoclass subgroups, the (0, 0, 0)+ set is selected in ITC83 in such a way that it corresponds to the general positions of an isoclass subgroup **S** with a primitive conventional cell. Under the heading 'Maximal non-isomorphic subgroups IIa' the HMS of **S** can be found. Depending on the centring type of the conventional cell of **G**, the index of **S** in **G** is 2, 3 or 4. Expressed in terms of the approach by Opechowski & Litvin (1977), the proposed OG-like symbols correspond to choosing **S** such that its HMS is obtained by replacing the first letter of the HMS of **G** by *P*.

In §3, first a list of the 58 OG superfamilies with a centred conventional cell that contain BW2 types will be given, together with the (0, 0, 0)+ sets corresponding to the two Litvin interpretations of the OG symbols and to our OG-like symbols. Next, the types of magnetic space groups for which the three symbols do not all agree will be listed together with the corresponding BNS symbol.

§4 investigates whether generators of the group can be read off from the OG symbols in cases where the conventional cell of **G** is primitive.

## 2. Definition of OG-like symbols for the BW2 types in the OG superfamilies with a centred conventional cell

The OG symbols for these BW2 types begin with a capital letter different from *P* with a subscript indicating the black–white lattice type, followed by a modified short point-group symbol, which we denote by *X*. According to Table 1, we can distinguish various cases.

(1) $C_{2c}X$ is obtained from its subgroup $CX$ with $\mathbf{c}^* = 2\mathbf{c}$ by adding the elements of $CX$ combined with the primed translation $\mathbf{c}'$.

(1*a*) $A_{2a}X$ is obtained from its subgroup $AX$ with $\mathbf{a}^* = 2\mathbf{a}$ by adding the elements of $AX$ combined with the primed translation $\mathbf{a}'$.

(2) $C_PX$ is obtained from its subgroup $PX$ by adding the elements of $PX$ combined with the primed translation $\frac{1}{2}(\mathbf{a}' + \mathbf{b}')$.

(2*a*) $A_PX$ is obtained from its subgroup $PX$ by adding the elements of $PX$ combined with the primed translation $\frac{1}{2}(\mathbf{b}' + \mathbf{c}')$.

(3) $C_IX$ is obtained from its subgroup $IX$ with $\mathbf{c}^* = 2\mathbf{c}$ by adding the elements of $IX$ combined with the primed translation $\mathbf{c}'$.

(3*a*) $A_IX$ is obtained from its subgroup $IX$ with $\mathbf{a}^* = 2\mathbf{a}$ by adding the elements of $IX$ combined with the primed translation $\mathbf{a}'$.

(4) $F_CX$ is obtained from its subgroup $CX$ by adding the elements of $CX$ combined with the primed translation $\frac{1}{2}(\mathbf{b}' + \mathbf{c}')$.

(4*a*) $F_AX$ is obtained from its subgroup $AX$ by adding the elements of $AX$ combined with the primed translation $\frac{1}{2}(\mathbf{a}' + \mathbf{b}')$.

(5) $I_PX$ is obtained from its subgroup $PX$ by adding the elements of $PX$ combined with the primed translation $\frac{1}{2}(\mathbf{a}' + \mathbf{b}' + \mathbf{c}')$.

(6) $R_RX$ is obtained from its subgroup $RX$ with $\mathbf{a}^* = \mathbf{b} + \mathbf{c}$, $\mathbf{b}^* = \mathbf{c} + \mathbf{a}$, $\mathbf{c}^* = \mathbf{a} + \mathbf{b}$ by adding the elements of $RX$ combined with the primed translation $\mathbf{a}' + \mathbf{b}' + \mathbf{c}'$.

Cases (1) and (2) appear in the monoclinic and the orthorhombic Bravais systems, cases (3) and (4) appear only in the orthorhombic one. Cases (1*a*), (2*a*), (3*a*) and (4*a*) appear only in crystal class *mm*2. Case (5) appears in the orthorhombic, tetragonal and cubic Bravais systems, case (6) appears only in the rhombohedral Bravais system.

The definitions (1)–(6) make sense only if the mentioned subgroups exist. ITC83 shows that this is the case except for the space-group types 108: *I*4*cm* and 140: *I*4/*mcm*; see also Table 2. Because in these two cases we not only have mirror planes *m* perpendicular to the third symmetry direction but also glide planes *c*, the OG superfamilies 108 and 140 will be called *I*4*cc* and *I*4/*mcc*, respectively. Definition (5) then becomes valid because space groups *P*4*cc* and *P*4/*mcc* exist but not space groups *P*4*cm* and *P*4/*mcm*.

ITC83 distinguishes three kinds of isoclass subgroups: IIa, IIb and IIc. The mentioned subgroups are of kind IIa in the cases (2), (2*a*), (4), (4*a*) and (5), of type IIb in the cases (3) and (3*a*). In the cases (1), (1*a*) and (6) they are of type IIb if *X* contains primes and of type IIc if *X* contains no primes.

Notice that we defined *X* to be a modified *short* point-group symbol. Let me explain the restriction to short symbols by considering an example: space group 67 has short symbol *Cmma* and full symbol $C\,2/m\,2/m\,2/a$. In the first two symmetry directions it has rotations 2 as well as screw rotations $2_1$. The subgroup 51 of index 2 has short symbol *Pmma* and full symbol $P\,2_1/m\,2/m\,2/a$. It has only $2_1$ in the first direction and only 2 in the second. Therefore the modified *full* point-group symbols do not agree for the space-group types 67 and 51.

The definitions given above show how the BW2 types in the OG superfamilies with a centred conventional cell can be obtained starting out from a monochrome type (if *X* contains no primes) or from a BW1 type (if *X* contains primes). The BW2 types are obtained from them by applying the primed translation given in the definitions (1)–(6). Notice that this step is similar to the construction of the BW2 types from their BNS symbol.

Notice also that the prescriptions (1)–(6) can be reformulated as follows: replace first the OG lattice symbol by the corresponding BNS lattice symbol $L_d$ according to Table 1. $L_dX$, where $L = P, C, A, I$ or $R$, is obtained from its subgroup $LX$ by adding the elements of $LX$ combined with the primed translation $\mathbf{t}'$, where $\mathbf{t} = \mathbf{a}^*/2, \mathbf{b}^*/2, \mathbf{c}^*/2$ if $d = a, b, c$; $\mathbf{t} = (\mathbf{b} + \mathbf{c})/2, (\mathbf{c} + \mathbf{a})/2, (\mathbf{a} + \mathbf{b})/2$ if $d = A, B, C$; $\mathbf{t} = (\mathbf{a}^* + \mathbf{b}^* + \mathbf{c}^*)/2$ if $d = I$; $\mathbf{t} = \mathbf{a}^*/2, \mathbf{b}^*/2$ or $\mathbf{c}^*/2$ if $d = s$.

## 3. Comparison of the various interpretations of OG symbols

In Table 2 the 58 OG superfamilies with a centred conventional cell that contain BW2 types are listed in the first column. Replacing the first letter in the HMS of column 1 by *P*,

**Table 3**
The orthorhombic OG superfamilies in which not all three OG symbols coincide.

| 1<br>Number and name of the OG superfamily | 2<br>Number of the BNS superfamily and standard BNS symbol | 3<br>Oriented BNS symbol | 4<br>OG-like symbol proposed | 5<br>OG symbol according to Litvin (1998) if different from column 4 | 6<br>OG symbol according to Opechowski & Guccione (1965) if different from column 4 |
|---|---|---|---|---|---|
| 45: $Iba2$ | 32: $P_Iba2$ | $P_Iba2$ | $I_Pba2$ | | $I_Pb'a'2$ |
| | 29: $P_Ica2_1$ | $P_Ibc2_1$ | $I_Pba'2'$ | | $I_Pb'a2'$ |
| | | $P_Ica2_1$ | $I_Pb'a2'$ | | $I_Pba'2'$ |
| | 27: $P_Icc2$ | $P_Icc2$ | $I_Pb'a'2$ | | $I_Pba2$ |
| 64: $Cmca$ | 57: $P_Bbcm$ | $P_Cmca$ | $C_Pmca$ | $C_Pmca'$ | $C_Pmca'$ |
| | 61: $P_Cbca$ | $P_Cbca$ | $C_Pm'ca$ | $C_Pm'ca'$ | $C_Pm'ca'$ |
| | 53: $P_Cmna$ | $P_Cmna$ | $C_Pmc'a$ | $C_Pmc'a'$ | $C_Pmc'a'$ |
| | 55: $P_Abam$ | $P_Cmcb$ | $C_Pmca'$ | $C_Pmca$ | $C_Pmca$ |
| | 62: $P_Cnma$ | $P_Cmnb$ | $C_Pmc'a'$ | $C_Pmc'a$ | $C_Pmc'a$ |
| | 54: $P_Acca$ | $P_Cbcb$ | $C_Pm'ca'$ | $C_Pm'ca$ | $C_Pm'ca$ |
| | 60: $P_Abcn$ | $P_Cbna$ | $C_Pm'c'a$ | $C_Pm'c'a'$ | $C_Pm'c'a'$ |
| | 56: $P_Accn$ | $P_Cbnb$ | $C_Pm'c'a'$ | $C_Pm'c'a$ | $C_Pm'c'a$ |
| 67: $Cmma$ | 67: $C_cmma$ | $C_cmma$ | $C_{2c}mma$ | | |
| | 64: $C_cmca$ | $C_ccmb$ | $C_{2c}m'ma$ | | |
| | 68: $C_ccca$ | $C_ccca$ | $C_{2c}m'm'a$ | | |
| | 51: $P_Cmma$ | $P_Cmma$ | $C_Pmma$ | $C_Pmma'$ | $C_Pmm'a$ |
| | | $P_Cmmb$ | $C_Pmma'$ | $C_Pmma$ | $C_Pmm'a'$ |
| | 57: $P_Abcm$ | $P_Cbma$ | $C_Pm'ma$ | $C_Pm'ma'$ | $C_Im'm'a$ |
| | | $P_Cmab$ | $C_Pmm'a'$ | $C_Pmm'a$ | $C_Pmma'$ |
| | 49: $P_Accm$ | $P_Cmaa$ | $C_Pmm'a$ | $C_Pmm'a'$ | $C_Pmma$ |
| | | $P_Cbmb$ | $C_Pm'ma'$ | $C_Pm'ma$ | $C_Pm'm'a'$ |
| | 54: $P_Bcca$ | $P_Cbaa$ | $C_Pm'm'a$ | $C_Pm'm'a'$ | $C_Pm'ma$ |
| | | $P_Cbab$ | $C_Pm'm'a'$ | $C_Pm'm'a$ | $C_Pm'ma'$ |
| | 74: $I_cmma$ | $I_cmma$ | $C_Imma$ | $C_Imma'$ | $C_Imm'a$ |
| | | $I_cmmb$ | $C_Imma'$ | $C_Imma$ | $C_Imm'a'$ |
| | 72: $I_abam$ | $I_ccma$ | $C_Im'ma$ | $C_Im'ma'$ | $C_Im'm'a$ |
| | | $I_ccmb$ | $C_Im'ma'$ | $C_Im'ma$ | $C_Im'm'a'$ |
| | | $I_cmca$ | $C_Imm'a$ | $C_Imm'a'$ | $C_Imma$ |
| | | $I_cmcb$ | $C_Imm'a'$ | $C_Imm'a$ | $C_Imma'$ |
| | 73: $I_cbca$ | $I_cbca$ | $C_Im'm'a$ | $C_Im'm'a'$ | $C_Im'ma$ |
| | | $I_cbcb$ | $C_Im'm'a'$ | $C_Im'm'a$ | $C_Im'ma'$ |
| 68: $Ccca$ | 54: $P_Ccca$ | $P_Ccca$ | $C_Pcca$ | | $C_Pc'ca'$ |
| | | $P_Cccb$ | $C_Pcca'$ | | $C_Pc'ca$ |
| | 60: $P_Bbcn$ | $P_Cnca$ | $C_Pc'ca$ | | $C_Pcca'$ |
| | | $P_Ccnb$ | $C_Pcc'a'$ | | $C_Pc'c'a$ |
| | 50: $P_Aban$ | $P_Ccna$ | $C_Pcc'a$ | | $C_Pc'c'a'$ |
| | | $P_Cncb$ | $C_Pc'ca'$ | | $C_Pcca$ |
| | 52: $P_Cnna$ | $P_Cnna$ | $C_Pc'c'a$ | | $C_Pcc'a'$ |
| | | $P_Cnnb$ | $C_Pc'c'a'$ | | $C_Pcc'a$ |
| 72: $Ibam$ | 55: $P_Ibam$ | $P_Ibam$ | $I_Pbam$ | | $I_Pb'a'm$ |
| | 57: $P_Ibcm$ | $P_Icam$ | $I_Pb'am$ | | $I_Pba'm$ |
| | | $P_Ibcm$ | $I_Pba'm$ | | $I_Pb'am$ |
| | 50: $P_Iban$ | $P_Iban$ | $I_Pbam'$ | | $I_Pb'a'm'$ |
| | 60: $P_Ibcn$ | $P_Ibcn$ | $I_Pba'm'$ | | $I_Pb'am'$ |
| | | $P_Ican$ | $I_Pb'am'$ | | $I_Pba'm'$ |
| | 49: $P_Iccm$ | $P_Iccm$ | $I_Pb'a'm$ | | $I_Pbam$ |
| | 56: $P_Iccn$ | $P_Iccn$ | $I_Pb'a'm'$ | | $I_Pbam'$ |
| 73: $Ibca$ | 61: $P_Ibca$ | $P_Ibca$ | $I_Pbca$ | | $I_Pb'c'a'$ |
| | | $P_Icab$ | $I_Pb'c'a'$ | | $I_Pbca$ |
| | 54: $P_Icca$ | $P_Icca$ | $I_Pb'ca$ | | $I_Pbc'a'$ |
| | | $P_Ibaa$ | $I_Pbc'a$ | | $I_Pb'ca'$ |
| | | $P_Ibcb$ | $I_Pbca'$ | | $I_Pb'c'a$ |
| | | $P_Ibab$ | $I_Pbc'a'$ | | $I_Pb'ca$ |
| | | $P_Iccb$ | $I_Pb'ca'$ | | $I_Pbc'a$ |
| | | $P_Icaa$ | $I_Pb'c'a$ | | $I_Pbca'$ |
| 74: $Imma$ | 51: $P_Imma$ | $P_Imma$ | $I_Pmma$ | $I_Pmma'$ | $I_Pmma'$ |
| | | $P_Immb$ | $I_Pmma'$ | $I_Pmma$ | $I_Pmma$ |
| | 62: $P_Inma$ | $P_Inma$ | $I_Pm'ma$ | $I_Pm'ma'$ | $I_Pm'ma'$ |
| | | $P_Imnb$ | $I_Pmm'a'$ | $I_Pmm'a$ | $I_Pmm'a$ |
| | 53: $P_Imna$ | $P_Imna$ | $I_Pmm'a$ | $I_Pmm'a'$ | $I_Pmm'a'$ |
| | | $P_Inmb$ | $I_Pm'ma'$ | $I_Pm'ma$ | $I_Pm'ma$ |
| | 52: $P_Inna$ | $P_Inna$ | $I_Pm'm'a$ | $I_Pm'm'a'$ | $I_Pm'm'a'$ |
| | | $P_Innb$ | $I_Pm'm'a'$ | $I_Pm'm'a$ | $I_Pm'm'a$ |

we obtain the HMS of a subgroup with a primitive conventional cell, the general-position coordinates of which play the role of the (0, 0, 0)+ set for the OG-like symbols that we propose. Column 2 gives the number and symbol of this subgroup. If the symbol does not have its standard form, the standard HMS has been added within parentheses. If the (0, 0, 0)+ set selected in ITC83 or in ITXC52 does not agree with the general-position coordinates of the subgroup given in column 2, this has been noted in columns 3 and 4, respectively.

Table 3 lists in column 1 the number and name of the orthorhombic OG superfamilies that contain types to which different OG symbols have been assigned. Column 2 gives the standard BNS symbols of the types in these OG superfamilies together with the number of the corresponding BNS superfamily. For different orientations of the group listed in column 2, column 3 gives the BNS symbol and column 4 the proposed OG-like symbol. If the symbols proposed by Litvin (1998) and by Opechowski & Guccione (1965) differ from the one given in column 4, they are listed in columns 5 and 6, respectively.

Note that the effect of the three interpretations of the OG symbols on the various types can be very different. Consider, for example, OG superfamily 45: whereas $I_Pba'2'$ and $I_Pb'a2'$ designate the same type in the proposed interpretation and in the interpretation of Opechowski & Guccione (1965), the one with standard BNS symbol $P_Ica2_1$, the types designated by $I_Pba2$ and $I_Pb'a'2$ are interchanged in the two interpretations.

The decisive advantage of the proposed OG-like symbols is that an unprimed (primed) symbol means that the corresponding generator is unprimed (primed), whereas in the two other interpretations the meaning of the symbols depends on the (0, 0, 0)+ sets selected in ITC83 and ITXC52, respectively. Note that the OG symbols based on the

**Table 4**
The non-orthorhombic OG superfamilies in which not all three OG symbols coincide.

| 1<br>Number and name of the OG superfamily | 2<br>Number of the BNS superfamily and standard BNS symbol | 3<br>OG-like symbol proposed | 4<br>OG symbol according to Litvin (1998) if different from column 3 | 5<br>OG symbol according to Opechowski & Guccione (1965) if different from column 3 |
|---|---|---|---|---|
| 108: $I4cm$ | 103: $P_I4cc$ | $I_P4cc$ | $I_P4cm$ | $I_P4c'm'$ |
| | 100: $P_I4bm$ | $I_P4c'c'$ | $I_P4c'm'$ | $I_P4cm$ |
| | 101: $P_I4_2cm$ | $I_P4'cc'$ | $I_P4'cm'$ | $I_P4'c'm$ |
| | 106: $P_I4_2bc$ | $I_P4'c'c$ | $I_P4'c'm$ | $I_P4'cm'$ |
| 140: $I4/mcm$ | 124: $P_I4/mcc$ | $I_P4/mcc$ | $I_P4/mcm$ | $I_P4/mcm$ |
| | 130: $P_I4/ncc$ | $I_P4/m'cc$ | $I_P4/m'cm$ | $I_P4/m'cm$ |
| | 135: $P_I4_2/mbc$ | $I_P4'/mc'c$ | $I_P4'/mc'm$ | $I_P4'/mc'm$ |
| | 132: $P_I4_2/mcm$ | $I_P4'/mcc'$ | $I_P4'/mcm'$ | $I_P4'/mcm'$ |
| | 127: $P_I4/mbm$ | $I_P4/mc'c'$ | $I_P4/mc'm'$ | $I_P4/mc'm'$ |
| | 138: $P_I4_2/ncm$ | $I_P4'/m'cc'$ | $I_P4'/m'cm'$ | $I_P4'/m'cm'$ |
| | 133: $P_I4_2/nbc$ | $I_P4'/m'c'c$ | $I_P4'/m'c'm$ | $I_P4'/m'c'm$ |
| | 125: $P_I4/nbm$ | $I_P4/m'c'c'$ | $I_P4/m'c'm'$ | $I_P4/m'c'm'$ |
| 206: $Ia\bar{3}$ | 205: $P_Ia\bar{3}$ | $I_Pa\bar{3}$ | | $I_Pa'\bar{3}$ |
| | | $I_Pa'\bar{3}'$ | | $I_Pa\bar{3}'$ |
| 214: $I4_132$ | 213: $P_I4_132$ | $I_P4_132$ | | $I_P4_1'32'$ |
| | 212: $P_I4_332$ | $I_P4_1'32'$ | | $I_P4_132$ |

(0, 0, 0)+ set selected in ITC83 differ in fewer cases from the proposed ones than the OG symbols based on ITXC52.

Table 4 lists in column 1 the number and name of the non-orthorhombic OG superfamilies that contain types to which different OG symbols have been assigned. Column 2 gives the standard BNS symbols of the types in these OG superfamilies together with the number of the corresponding BNS superfamily; column 3 gives the corresponding OG-like symbol. If the symbols proposed by Litvin (1998) and by Opechowski & Guccione (1965) differ from the one given in column 3, they are listed in columns 4 and 5, respectively.

Figs. 2 and 3 illustrate the first and the third case from OG superfamily 108: $I4cm$. The groups shown have in symmetry direction 2 (horizontal and vertical) $c$-glide planes. In symmetry direction 3 (diagonal) Fig. 2 has $c$-glide planes and Fig. 3 has $c'$-glide planes, as indicated in the proposed OG-like symbol. The symmetry elements present in symmetry direction 2 show that the OG symbol of Opechowski & Guccione (1965) cannot be interpreted in this simple way; the symmetry elements present in symmetry direction 3 also show that the OG symbol of Litvin (1998) cannot be interpreted in this simple way.

Note that the OG superfamilies 80 and 98 do not appear in Table 4; although the (0, 0, 0)+ set selected in ITXC52 differs from the one in ITC83 as indicated in Table 2, this does not affect the interpretation of the OG symbols according to the procedure described by Opechowski & Litvin (1977). Note also that the different assignments of OG symbols depending on whether they are interpreted according to ITXC52 or ITC83 (last two columns of Tables 3 and 4) agree with Table 2 of Litvin (1998).

## 4. Definition of OG-like symbols for the BW2 types in the OG superfamilies with a primitive conventional cell

If the conventional cell of **G** is primitive, which is the case in 287 among the 517 BW2 types, the OG symbols according to Opechowski & Guccione (1965) and according to Litvin (1998) coincide because the positions in a cell are then not split into two, three or four sets, as for centred cells. For six types these authors do not derive the OG symbol from the symbol of the OG superfamily to which the type belongs. We propose OG-like symbols that differ as follows from theirs: the BW2 type in superfamily $P3_1$ will be called $P_{2c}3_1$, the one in $P3_2$ will be called $P_{2c}3_2$, *i.e.* $P_{2c}3_1$ and $P_{2c}3_2$ exchange their meaning, similarly $P_{2c}3_112 \leftrightarrow P_{2c}3_212$ and $P_{2c}3_121 \leftrightarrow P_{2c}3_221$.

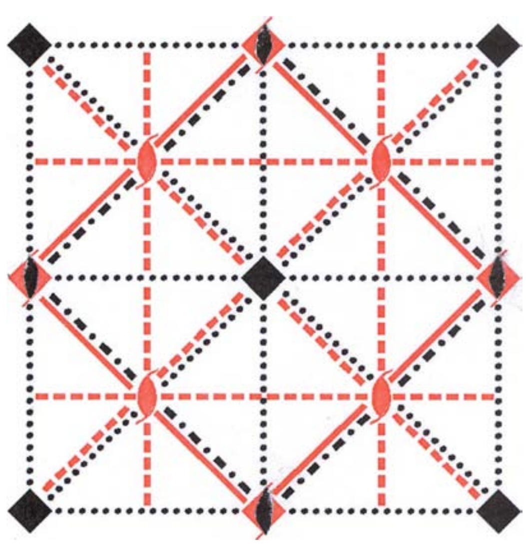

**Figure 2**
Symmetry diagram for the space group with BNS symbol $P_I4cc$. OG-like symbol proposed: $I_P4cc$. OG symbol according to Opechowski & Guccione (1965): $I_P4c'm'$, according to Litvin (1998): $I_P4cm$.

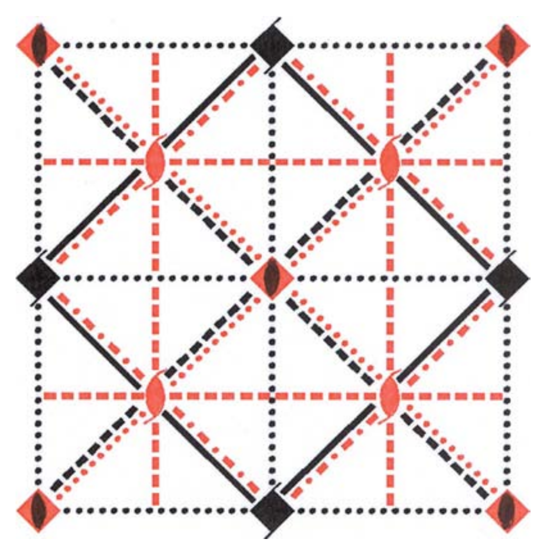

**Figure 3**
Symmetry diagram for the space group with BNS symbol $P_I4_2cm$. OG-like symbol proposed: $I_P4'cc'$. OG symbol according to Opechowski & Guccione (1965): $I_P4'c'm$, according to Litvin (1998): $I_P4'cm'$.

The meaning of the OG-like symbols for the BW2 types in the OG superfamilies with a primitive conventional cell can then be defined as follows:

(7*a*) $P_{2a}X$ is obtained from its subgroup $PX$ with $\mathbf{a}^* = 2\mathbf{a}$ by adding the elements of $PX$ combined with the primed translation $\mathbf{a}'$.

(7*b*) $P_{2b}X$ is obtained from its subgroup $PX$ with $\mathbf{b}^* = 2\mathbf{b}$ by adding the elements of $PX$ combined with the primed translation $\mathbf{b}'$.

(7*c*) $P_{2c}X$ is obtained from its subgroup $PY$ with $\mathbf{c}^* = 2\mathbf{c}$ by adding the elements of $PY$ combined with the primed translation $\mathbf{c}'$. $Y$ differs from $X$ in that $3_1$ is replaced by $3_2$, $3_2$ by $3_1$, $4_2$ by $4_1$, $6_2$ by $6_1$, and $6_4$ by $6_2$.

(8) $P_CX$ (monoclinic and orthorhombic cases) and $P_PX$ (tetragonal cases) are obtained from their subgroup $CX$ with $\mathbf{a}^* = 2\mathbf{a}$ and $\mathbf{b}^* = 2\mathbf{b}$ by adding the elements of $CX$ combined with the primed translation $\mathbf{a}'$.

$P_AX$ (orthorhombic cases) is obtained from its subgroup $AX$ with $\mathbf{b}^* = 2\mathbf{b}$ and $\mathbf{c}^* = 2\mathbf{c}$ by adding the elements of $AX$ combined with the primed translation $\mathbf{c}'$.

(9) $P_FX$ (orthorhombic and cubic cases) and $P_IX$ (tetragonal cases) are obtained from their subgroup $FY$ with $\mathbf{a}^* = 2\mathbf{a}$, $\mathbf{b}^* = 2\mathbf{b}$ and $\mathbf{c}^* = 2\mathbf{c}$ by adding the elements of $FY$ combined with the primed translation $\mathbf{c}'$. $Y$ differs from $X$ in that $4_2$ is replaced by $4_1$ and $n$ by $d$.

Notice that, according to Table 1, case (7) appears in all Bravais systems except the rhombohedral and cubic ones. The subgroups mentioned under (7)–(9) are either of type IIb or IIc; all those mentioned under (9) and the non-tetragonal ones mentioned under (8) are of type IIb. The anorthic, monoclinic and orthorhombic subgroups mentioned under (7) are of type IIc if $X$ is unprimed and of type IIb otherwise.

The definitions given above show how the BW2 types in the OG superfamilies with a primitive conventional cell can be obtained starting out from a monochrome type (if $X$ contains no primes) or from a BW1 type (if $X$ contains primes). The BW2 type is then obtained by applying the primed translation given in the definitions (7)–(9).

The change of six symbols proposed above has the consequence that $Y$ defined in (7*c*) differs from $X$ also if it contains $3_1$ or $3_2$. It seems to us more satisfactory to state that a phenomenon that appears for four- and sixfold screw rotations occurs also for the threefold ones instead of hiding this fact by abandoning the principle by which the symbols for the BW2 types are constructed from the symbol of their superfamily.

## 5. Discussion

OG-like symbols have been defined in §§2 and 4 by the prescriptions (1)–(9), which show how the 571 BW2 types can be constructed starting from an ordinary space group (or a BW1 group) if the OG-like symbol does not (does) contain primes. The BW2 type is then obtained by applying the primed translation given in the prescriptions (1)–(9). Notice that this step is similar to the construction of the BW2 types from their BNS symbol. The advantages of our OG-like symbols compared to the OG symbols are: their meaning is defined by the prescriptions (1)–(9), independent of any choice of (0, 0, 0)+ set; the OG superfamily to which the type belongs can immediately be read off the OG symbol without any exceptions.

**Table 5**
Change of standard HMSs in ITC95.

| Number of space group | Old standard HMS | Alternative HMS | New standard HMS |
|---|---|---|---|
| 39 | *Abm*2 | *Acm*2 | *Aem*2 |
| 41 | *Aba*2 | *Aca*2 | *Aea*2 |
| 64 | *Cmca* | *Cmcb* | *Cmce* |
| 67 | *Cmma* | *Cmmb* | *Cmme* |
| 68 | *Ccca* | *Cccb* | *Ccce* |

In order to compare the OG-like symbols with the symbols proposed by Opechowski & Guccione (1965) and those proposed by Litvin (1998), the definition of the OG-like symbols was also formulated in §3 in the language of (0, 0, 0)+ sets.

In the fourth edition of Volume A of *International Tables for Crystallography* (1995), abbreviated as ITC95, a new graphical symbol *e* was introduced for double glide planes and new HMSs were proposed for the space groups 39, 41, 64, 67 and 68, as shown in Table 5.

This change of the HMS must not be made in the OG symbols, because an *e* in an OG symbol does not tell us which of the two glide planes is unprimed.

We stressed that for the BNS symbols there is no doubt concerning their interpretation. The description of how a BW2 type is obtained from the monochrome type denoted by the BNS symbol without its centring subscript is simpler than the prescriptions (1)–(9) given above. Generators can in all cases be read off the BNS symbol directly, whereas in the case of OG-like symbols certain screw rotations and *n*-glide planes must be replaced beforehand according to the prescriptions (7*c*) and (9). Further advantages of the BNS symbols have been pointed out by Grimmer (2009). Why should we then use OG symbols instead in certain applications?

One aspect is that all the types of an OG superfamily except the grey one are isomorphic. It follows that the OG symbols of the black–white types are closely connected with the information given on the subgroups **H** with index 2 in **G** listed in ITC83 (and its more recent editions) under I, IIa, IIb and IIc. For the BW1 types, **H** is isotranslational (type I) and for the BW2 types **H** is isoclass (type II). Consider the various values of $n$ given in Table 1. If $n = 0$ the group **G** and its subgroup **H** consisting of the unprimed operations have the same conventional cell, *i.e.* **H** is of type IIa. If $n = 1$ then **H** is of type IIc (or IIb), *i.e.* **H** has a larger conventional cell than **G** and is (or is not) isomorphic to **G**. If $n = 2$ or 3 then **H** is of type IIb. More detailed results have been given in §§2 and 4.

Another aspect is that there is a one-to-one correspondence between the one-dimensional real representations of each of the 230 space-group types and the monochrome, BW1 and BW2 types in the corresponding OG superfamily, as pointed out by Bertaut (1968). In the one-dimensional real representations the characters are either +1 or −1. The monochrome type corresponds to the trivial representation, in which all characters are +1. The character is 1 for unprimed and −1 for primed symmetry operations in the black–white types.

## 6. Conclusions

For the OG superfamilies with a centred conventional cell, OG-like symbols for the magnetic space-group types containing primed translations have been proposed for which an unprimed (primed) symmetry element appearing in the symbol denotes an unprimed (primed) generator of the group. This is in contrast to the OG symbols introduced by Opechowski & Guccione (1965) and those proposed by Litvin (1998), the meaning of which depends on the (0, 0, 0)+ set selected in ITXC52 and ITC83, respectively. The three symbols differ in several cases.

Our approach required renaming the OG superfamilies 108 ($I4cm \rightarrow I4cc$) and 140 ($I4/mcm \rightarrow I4/mcc$). It also required keeping for the OG superfamilies 39, 41, 64, 67 and 68 the standard symbols of the corresponding space groups before the changes made in ITC95. Whereas it certainly was a good idea to introduce a new graphical symbol for double glide planes, which appear in 17 space-group types, changing the HMSs for five of these types hides the relation between these five types and the corresponding types with a primitive conventional cell.

For the OG superfamilies with a primitive conventional cell, generators of the group can also be read off the OG-like symbol except for:

(1) $P_{2c}X$ if $X$ contains screw rotations $3_1$, $3_2$, $4_2$, $6_2$ or $6_4$, in which cases the generators are obtained after replacing $3_1$ by $3_2$, $3_2$ by $3_1$, $4_2$ by $4_1$, $6_2$ by $6_1$, and $6_4$ by $6_2$; and

(2) $P_FX$ and $P_IX$ if $X$ contains $4_2$ or $n$, in which cases the generators are obtained after replacing $4_2$ by $4_1$ and $n$ by $d$.

## References


Belov, N. V., Neronova, N. N. & Smirnova, T. S. (1957*a*). *Kristallografiya*, **2**, 315–325.

Belov, N. V., Neronova, N. N. & Smirnova, T. S. (1957*b*). *Sov. Phys. Crystallogr.* **2**, 311–322.

Bertaut, E. F. (1968). *Acta Cryst.* A**24**, 217–231.

Bertaut, E. F. (1975). *Ann. Phys.* **9**, 93–108.

Bertaut, E. F. (1977). *Ann. Phys.* **2**, 127–131.

Borovik-Romanov, A. S. & Grimmer, H. (2003). *International Tables for Crystallography*, Vol. D, edited by A. Authier, pp. 105–149. Dordrecht: Kluwer Academic Publishers.

Burzlaff, H. & Zimmermann, H. (1983). *International Tables for Crystallography*, Vol. A, *Space-Group Symmetry*, Section 12.3, edited by Th. Hahn. Dordrecht: D. Reidel Publishing Company.

Grimmer, H. (2009). *Acta Cryst.* A**65**, 145–155.

Hermann, C. (1928). *Z. Kristallogr.* **68**, 257–287.

Hermann, C. (1931). *Z. Kristallogr.* **76**, 559–561.

*International Tables for Crystallography* (1983). Vol. A, *Space-Group Symmetry*, 1st ed., edited by Th. Hahn. Dordrecht: Reidel Publishing Company.

*International Tables for Crystallography* (1995). Vol. A, *Space-Group Symmetry*, 4th ed., edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers.

*International Tables for X-ray Crystallography* (1952). Vol. I. *Symmetry Groups*, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press.

Litvin, D. B. (1998). *Acta Cryst.* A**54**, 257–261.

Litvin, D. B. (2001). *Acta Cryst.* A**57**, 729–730.

Litvin, D. B. (2008). *Acta Cryst.* A**64**, 419–424.

Mauguin, Ch. (1931). *Z. Kristallogr.* **76**, 542–558.

Opechowski, W. & Guccione, R. (1965). *Magnetism*, edited by G. T. Rado & H. Suhl, Vol. II, Part A, pp. 105–165. New York: Academic Press.

Opechowski, W. & Litvin, D. B. (1977). *Ann. Phys.* **2**, 121–125.