RESEARCH PAPERS

Acta Cryst. (1998). A**54**, 257–261

On Opechowski–Guccione Magnetic Space-Group Symbols

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(Received 27 May 1997; accepted 29 September 1997)

Abstract

The interpretation of Opechowski–Guccione magnetic space-group symbols is based, in part, on the printed coordinate triplets of the general positions of space groups given in *International Tables for X-ray Crystallography* (1952), Vol. 1. (Birmingham: Kynoch Press). This volume has been replaced by *International Tables for Crystallography* (1983), Vol. A (Dordrecht: Kluwer Academic Publishers), where changes have been made in these printed coordinate triplets of the general positions. The use of the original Opechowski–Guccione symbols with this latter volume leads to misinterpretations and ambiguities. In this paper, all cases where the changes in the printed coordinate triplets of the general positions have the consequence of changing the meaning of Opechowski–Guccione symbols for magnetic space groups are tabulated. In addition, the changes to magnetic space-group symbols owing to the change in the notation for the two cubic crystal classes $m\bar{3}$ and $m\bar{3}m$, which now contain the symbol $\bar{3}$ instead of 3, and the consequences of the introduction of the symbol *e* into the symbols for space groups are discussed.

1. Introduction

A list of symbols for all 1191 types (classes) of magnetic space groups has been given by Opechowski & Guccione (1965) (see also Opechowski, 1986). [This number plus 230 space-group types and 230 types of groups which are the direct product of a space group and the time-inversion group gives a total of 1651 types of groups (Belov *et al.*, 1957).] This list of 1191 symbols will be referred to as the OG symbols. This list consists of a listing of a symbol for one representative magnetic space group from each of the 1191 types. To uniquely specify the meaning of these 1191 symbols for magnetic space groups requires a specification of a symbol for one representative space group from each of the 230 types of space groups. The specification of these 230 symbols for space groups was made in conjunction with Vol. I of *International Tables for X-ray Crystallography* (1952) (abbreviated here as *ITC*52). In particular, this specification of the space-group symbols was based on the specific form of the coordinate triplets of the set of general positions explicitly printed in *ITC*52. Consequently, the meaning of the symbols for the magnetic space groups listed by Opechowski & Guccione (1965) depend on the coordinate triplets of the general positions explicitly printed in *ITC*52.

*ITC*52 has been replaced by Vol. A of *International Tables for Crystallography* (1983) (abbreviated here as *ITC*83). One finds that, for some space groups, the set of coordinate triplets of the general positions explicitly printed in *ITC*83 differ from those explicitly printed in *ITC*52. As a consequence, if one attempts to interpret OG symbols using *ITC*83, one will, in many cases, misinterpret the meaning of the symbol. In some cases, this misinterpretation will not lead to erroneous conclusions as to the number of the magnetic space-group types nor to the validity of the list of OG symbols as a list of one magnetic space group from each type of magnetic space group. However, in other cases, this misinterpretation will lead, as we show below, to erroneous conclusions. In addition, the correspondence, given by Opechowski & Guccione (1965), of the OG symbols with that set of symbols given by Belov *et al.* (1957)† (referred to here as BNS symbols) would also be called into question. In terms of magnetic structure analysis, the OG symbol for the magnetic space group of a particular magnetic structure can be different depending on whether one uses *ITC*52 or *ITC*83 to interpret the meaning of the OG symbols.

In §2, we review the conventions used by Opechowski & Guccione (1965) in deriving their list of symbols for magnetic space-group types. Of central importance is their convention concerning the choice of the representative space group from each space-group type, its symbol and the choice of a set of coset repre-

† In Opechowski & Guccione (1965), in the listing of the BNS symbols corresponding to OG symbols, there are errors in some BNS symbols. Corrections are given in Opechowski & Litvin (1977). There is one misprint: The symbol $C_I m'm'm'$ should read $C_I m'mm'$ as is listed in Opechowski (1986).

sentatives of the translation subgroup in this space group. In §3, we show how the use of *ITC*83 in place of *ITC*52 leads to differences in the interpretation of the OG symbols. We then show the correspondence between OG symbols based on *ITC*52 and OG symbols based on *ITC*83.

In §4, we discuss changes to the list of OG symbols due to the changes in *ITC*83 to symbols of cubic space-group types. The cubic space-group types numbered 200–206 and 221–230 belonging to the two cubic crystal classes $m\bar{3}$ and $m\bar{3}m$ now contain the symbol $\bar{3}$ instead of 3. We also discuss the implications of the introduction of the symbol *e* into the Hermann–Mauguin symbol of five space-group types.

2. Opechowski & Guccione conventions

Here, in order to distinguish group symbols from group-type symbols, the group symbols are given in ***bold italic*** type.

Magnetic space groups $\boldsymbol{M}$ are divided into two types: $\boldsymbol{M_T}$ groups with a translational subgroup with no primed translations, *i.e.* no translation is coupled with the time-inversion operation, and $\boldsymbol{M_R}$ groups with a translational subgroup with one half of the translations primed. As differences in interpretation of the OG symbols have to do only with magnetic space groups of the type $\boldsymbol{M_R}$, we review here the steps followed to obtain an OG symbol for such groups.

(i) One representative space group $\boldsymbol{F}$ is chosen from each of the 230 types of space groups. For each of the 230 types *F* of space groups, one finds in *ITC* (in both *ITC*52 and *ITC*83) a specification of the coordinate system used and in terms of that coordinate system a specification of the lattice (subgroup of translations) $\boldsymbol{T}$ of one space group $\boldsymbol{F}$ belonging to type *F*. In addition, indirectly, a specification is given of a set of *n* coset representatives of $\boldsymbol{T}$ in $\boldsymbol{F}$, where *n* is the index of $\boldsymbol{T}$ in $\boldsymbol{F}$. What is specified are the coordinates of *n*, or small multiple of *n*, equivalent positions. From among these, there is a printed list for exactly *n* positions. This printed list uniquely determines a set of *n* coset representatives of $\boldsymbol{T}$ in $\boldsymbol{F}$. The representative space group $\boldsymbol{F}$ is defined by the lattice specification and this set of *n* coset representatives of $\boldsymbol{T}$ in $\boldsymbol{F}$ specified by the printed set of coordinate triplets of *n* equivalent general positions. The symbol for this representative space group $\boldsymbol{F}$ is taken to be identical with the symbol for the type *F* to which $\boldsymbol{F}$ belongs printed at the top of the page in *ITC*.

For example, consider the space-group-type No. 68, *F* = *Ccca* (*International Tables for X-ray Crystallography* (1969, p. 157). The lattice is

$$\boldsymbol{C} = \langle (1|\tfrac{1}{2}\tfrac{1}{2}0), (1|\tfrac{1}{2}\tfrac{\bar{1}}{2}0), (1|001)\rangle.$$

The coordinate triplets of the general positions printed on page 157 of *ITC*52 are:

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

Consequently, the coset representative of the translational subgroup $\boldsymbol{T} = \boldsymbol{C}$ in the representative space group $\boldsymbol{F} = \boldsymbol{Ccca}$ are:

$$\begin{array}{llll} (1|000), & (2_z|000), & (2_y|000)\,, & (2_x|000), \\ (\bar{1}|0\tfrac{1}{2}\tfrac{1}{2}), & (m_z|0\tfrac{1}{2}\tfrac{1}{2}), & (m_y|0\tfrac{1}{2}\tfrac{1}{2}), & (m_x|0\tfrac{1}{2}\tfrac{1}{2}). \end{array} \qquad (1)$$

The translational subgroup $\boldsymbol{T} = \boldsymbol{C}$ and this set of coset representatives of $\boldsymbol{T}$ in $\boldsymbol{F}$ uniquely define the representative space group $\boldsymbol{F} = \boldsymbol{Ccca}$.

There does exist a set of rules by which one can determine from the space-group-type symbol *F* the lattice $\boldsymbol{T}$ and a set of coset representatives of $\boldsymbol{T}$ in a space group $\boldsymbol{F}$ belonging to type *F* (Section 12.3 of *ITC*83). However, following this set of rules gives rise, in some cases, to a set of coordinate triplets of the general positions that differ from those printed in *ITC* (as explicitly stated in Section 12.3 of *ITC*83). To avoid this ambiguity, Opechowski & Guccione (1965) follow the convention of always using the set of coset representatives implied by the set of coordinate triplets of the general positions printed in *ITC*52.

(ii) A magnetic space group $\boldsymbol{M_R}$ that belongs to the family of a space group $\boldsymbol{F}$ has the form

$$\boldsymbol{M_R} = \boldsymbol{D_R} + (\boldsymbol{F} - \boldsymbol{D_R})1',$$

where $\boldsymbol{D_R}$ is an equi-class subgroup of index 2 of $\boldsymbol{F}$ and $1'$ is time inversion. An OG symbol, as we show below, specifies both $\boldsymbol{D_R}$ and $\boldsymbol{F}$, and consequently is used as a symbol of the subgroup $\boldsymbol{D_R}$, the corresponding magnetic space group $\boldsymbol{M_R}$ and also as a symbol of the type M_R of magnetic space groups to which that group $\boldsymbol{M_R}$ belongs.

For a given representative space group $\boldsymbol{F}$, one selects one of the subgroups $\boldsymbol{T^D}$ of index 2 in $\boldsymbol{T}$. One then specifies one translation t_α that belongs to $\boldsymbol{T}$ but not to $\boldsymbol{T^D}$, and therefore $\boldsymbol{T} = \boldsymbol{T^D} + t_\alpha \boldsymbol{T^D}$. Each subgroup $\boldsymbol{D_R}$ of index 2 in $\boldsymbol{F}$, which has the translational subgroup $\boldsymbol{T^D}$ can then be specified by a set of coset representatives of $\boldsymbol{T^D}$ in $\boldsymbol{D_R}$. This set of coset representatives is obtained from the set of coset representatives of $\boldsymbol{T}$ in $\boldsymbol{F}$ (implied by the set of coordinate triplets of the general positions printed in *ITC*) by multiplying by t_α some, or possibly none, of the coset representatives.

Each subgroup $\boldsymbol{D_R}$ of $\boldsymbol{F}$ is assigned an OG symbol in two steps. One starts with the symbol for *F*. Then: (*a*) the translational subgroup symbol for $\boldsymbol{T}$ in the symbol of $\boldsymbol{F}$ is replaced by the symbol of the lattice $\boldsymbol{T^D}$ of $\boldsymbol{D_R}$; and (*b*) if a number or letter associated with a coset representative of $\boldsymbol{T}$ in $\boldsymbol{F}$ appears in the symbol of $\boldsymbol{F}$ and this coset representative has been multiplied by t_α then a prime is attached to that number or letter.

For example, consider the representative space group $\boldsymbol{F} = \boldsymbol{Ccca}$ defined above. We select the subgroup $\boldsymbol{T^D} = \boldsymbol{C_P}$ of $\boldsymbol{T} = \boldsymbol{C}$:

$$\boldsymbol{C_P} = \langle(1|100), (1|010), (1|001)\rangle \tag{2}$$

and $t_\alpha = (1|\frac{1}{2}\frac{1}{2}0)$, then $\boldsymbol{C} = \boldsymbol{C_P} + (1|\frac{1}{2}\frac{1}{2}0)\boldsymbol{C_P}$. One of the subgroups $\boldsymbol{D_R}$ of $\boldsymbol{Ccca}$ is that subgroup whose translational subgroup is $\boldsymbol{C_P}$ and whose set of coset representatives of $\boldsymbol{C_P}$ in $\boldsymbol{D_R}$ is the same as the set of coset representatives, see (1), of $\boldsymbol{C}$ in $\boldsymbol{F} = \boldsymbol{Ccca}$, *i.e.* none of the coset representatives are multiplied by t_α. Consequently, the symbol for this subgroup $\boldsymbol{D_R}$ is $\boldsymbol{C_Pcca}$. This symbol also specifies $\boldsymbol{F} = \boldsymbol{Ccca}$ and the magnetic space group $\boldsymbol{M_R} = \boldsymbol{C_Pcca}$.

A second subgroup $\boldsymbol{D_R}$ of $\boldsymbol{Ccca}$ with the translational subgroup $\boldsymbol{C_P}$ is specified by the following set of coset representatives of $\boldsymbol{C_P}$ in $\boldsymbol{D_R}$:

$$\begin{array}{llll} (1|000), & (2_z|000), & (2_y|\frac{1}{2}\frac{1}{2}0), & (2_x|\frac{1}{2}\frac{1}{2}0), \\ (\bar{1}|\frac{1}{2}0\frac{1}{2}), & (m_z|\frac{1}{2}0\frac{1}{2}), & (m_y|0\frac{1}{2}\frac{1}{2}), & (m_x|0\frac{1}{2}\frac{1}{2}). \end{array} \tag{3}$$

Because $(m_z|\frac{1}{2}0\frac{1}{2}) = (1|\frac{1}{2}\frac{1}{2}0)(m_z|0\frac{1}{2}\frac{1}{2}) = (1|t_\alpha)(m_z|0\frac{1}{2}\frac{1}{2})$, modulo translations of $\boldsymbol{T^D}$, while $(m_y|0\frac{1}{2}\frac{1}{2})$ and $(m_x|0\frac{1}{2}\frac{1}{2})$ have not been multiplied, see (1), by t_α, the symbol for this subgroup $\boldsymbol{D_R}$ is $\boldsymbol{C_Pcca'}$.

There is a total of eight subgroups $\boldsymbol{D_R}$ of $\boldsymbol{F} = \boldsymbol{Ccca}$ with a translational subgroup $\boldsymbol{T^D} = \boldsymbol{C_P}$. These fall into four groups of two, each pair representing a pair of subgroups $\boldsymbol{D_R}$ belonging to the same type of space group. These pairs of groups are given in the first column of Table 1 with the space-group type given in column 2.

As symbols for magnetic space groups, each pair of symbols are of magnetic space groups $\boldsymbol{M_R}$ belonging to the same type M_R. [If two subgroups $\boldsymbol{D_R}$ of $\boldsymbol{F}$ have a common translational subgroup and belong to the same class of space groups, then the two corresponding magnetic space groups $\boldsymbol{M_R}$ belong to the same type of magnetic space group (see Opechowski, 1986).] Consequently, one finds only the first symbol from each pair listed among the OG symbols.

3. Impact of *ITC*83

In *ITC*83, one finds that some sets of coordinate triplets of general positions explicitly printed are different from those printed in *ITC*52. For example, the coordinate triplets of the general positions explicitly print in the case of space-group-type No. 68, $F = Ccca$ on page 303 in *ITC*83 are:

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

Table 1. *Symbols for the subgroups* $\boldsymbol{D_R}$ *of* $\boldsymbol{F} = \boldsymbol{Ccca}$ *with translational subgroup* $\boldsymbol{T^D} = \boldsymbol{C_P}$ *using the conventions of Opechowski & Guccione (1965) and ITC52 and ITC83*

*ITC*52		$\boldsymbol{D_R}$ type	*ITC*83	
$\boldsymbol{C_Pcca}$	$\boldsymbol{C_Pc'c'a'}$	*Pban*	$\boldsymbol{C_Pcc'a}$	$\boldsymbol{C_Pc'ca'}$
$\boldsymbol{C_Pc'ca}$	$\boldsymbol{C_Pc'ca'}$	*Pcca*	$\boldsymbol{C_Pcca}$	$\boldsymbol{C_Pcca'}$
$\boldsymbol{C_Pcca'}$	$\boldsymbol{C_Pc'c'a}$	*Pbcn*	$\boldsymbol{C_Pc'ca}$	$\boldsymbol{C_Pcc'a'}$
$\boldsymbol{C_Pcc'a'}$	$\boldsymbol{C_Pcc'a}$	*Pnna*	$\boldsymbol{C_Pc'c'a}$	$\boldsymbol{C_Pc'c'a'}$

Consequently, from *ITC*83 and the conventions of §2, the coset representatives of the translational subgroup $\boldsymbol{T} = \boldsymbol{C}$ in the representative space group $\boldsymbol{F} = \boldsymbol{Ccca}$ are:

$$\begin{array}{llll} (1|000), & (2_z|\frac{1}{2}\frac{1}{2}0), & (2_y|000), & (2_x|\frac{1}{2}\frac{1}{2}0), \\ (\bar{1}|0\frac{1}{2}\frac{1}{2}), & (m_z|\frac{1}{2}0\frac{1}{2}), & (m_y|0\frac{1}{2}\frac{1}{2}), & (m_x|\frac{1}{2}0\frac{1}{2}). \end{array} \tag{4}$$

We consider those subgroups of index 2 of $\boldsymbol{F} = \boldsymbol{Ccca}$ with the translational subgroup $\boldsymbol{T^D} = \boldsymbol{C_P}$ and take $t_\alpha = (1|\frac{1}{2}\frac{1}{2}0)$. One of the subgroups $\boldsymbol{D_R}$ of $\boldsymbol{Ccca}$ is that subgroup whose translational subgroup is $\boldsymbol{C_P}$ and whose set of coset representatives of $\boldsymbol{C_P}$ in $\boldsymbol{D_R}$ are the same as the set of coset representatives, see (4), of $\boldsymbol{C}$ in $\boldsymbol{F} = \boldsymbol{Ccca}$, *i.e.* none of the coset representatives are multiplied by t_α. Consequently, the symbol for this subgroup $\boldsymbol{D_R}$ is $\boldsymbol{C_Pcca}$. This symbol also specifies $\boldsymbol{F} = \boldsymbol{Ccca}$ and the magnetic space group $\boldsymbol{M_R} = \boldsymbol{C_Pcca}$.

A second subgroup $\boldsymbol{D_R}$ of $\boldsymbol{Ccca}$ with the translational subgroup $\boldsymbol{C_P}$ is specified by the following set of coset representatives of $\boldsymbol{C_P}$ in $\boldsymbol{D_R}$:

$$\begin{array}{llll} (1|000), & (2_z|\frac{1}{2}\frac{1}{2}0), & (2_y|000), & (2_x|\frac{1}{2}\frac{1}{2}0), \\ (\bar{1}|0\frac{1}{2}\frac{1}{2}), & (m_z|0\frac{1}{2}\frac{1}{2}), & (m_y|0\frac{1}{2}\frac{1}{2}), & (m_x|0\frac{1}{2}\frac{1}{2}). \end{array}$$

Because $(m_z|0\frac{1}{2}\frac{1}{2}) = (1|\frac{1}{2}\frac{1}{2}0)(m_z|\frac{1}{2}0\frac{1}{2}) = (1|t_\alpha)(m_z|\frac{1}{2}0\frac{1}{2})$, modulo translations of $\boldsymbol{T^D}$, while $(m_y|0\frac{1}{2}\frac{1}{2})$ and $(m_x|0\frac{1}{2}\frac{1}{2})$ have not been multiplied by t_α, the symbol for subgroup $\boldsymbol{D_R}$ is $\boldsymbol{C_Pcca'}$.

There is a total of eight subgroups $\boldsymbol{D_R}$ of $\boldsymbol{F} = \boldsymbol{Ccca}$ with a translational subgroup $\boldsymbol{T^D} = \boldsymbol{C_P}$. These fall into four groups of two, each pair representing a pair of subgroups $\boldsymbol{D_R}$ belonging to the same type of space group. These pairs of groups are given in the third column of Table 1 with the space-group type given in column 2.

From Table 1, one can see the differences in the interpretations of OG symbols when using *ITC*83 instead of *ITC*52. The symbols $\boldsymbol{C_Pcca}$ and $\boldsymbol{C_Pcca'}$ are, using *ITC*52, symbols for two subgroups of index 2 of $\boldsymbol{F} = \boldsymbol{Ccca}$, which belong to two *different* types of space groups, and are symbols for two magnetic groups $\boldsymbol{M_R}$, which belong to two *different* types of magnetic space groups. These same two symbols, $\boldsymbol{C_Pcca}$ and $\boldsymbol{C_Pcca'}$, are, using *ITC*83, symbols for two subgroups of index 2 of $\boldsymbol{F} = \boldsymbol{Ccca}$, which belong to the same type of space group, and are symbols for two magnetic groups $\boldsymbol{M_R}$, which belong to the same type of magnetic space group. Using *ITC*83, one could then erroneously conclude that the list of OG symbols (Opechowski & Guccione, 1965; Opechowski, 1986) contains redundant magnetic space-group types. Also, since the space-group types of the space groups $\boldsymbol{D_R}$ associated with these symbols are, according to *ITC*83, different from the space-group types according to *ITC*52, one could then also erroneously conclude that the correspondence of the OG symbols and the BNS symbols given by Opechowski & Guccione (1965) are not correct. These differences in interpretation of OG symbols are due to the changes made in *ITC*83 to the printed list of coordinate triplets of general positions for the space-group type *Ccca* and the subsequent differences, see (1) and (4), in the coset representatives of the translational subgroup $\boldsymbol{T} = \boldsymbol{C}$ in $\boldsymbol{F} = \boldsymbol{Ccca}$.

In Table 2, for all space-group types *F* where the printed coordinate triplets of general positions differ in *ITC*52 and *ITC*83 and those cases that lead to different OG symbols, we list the subgroups $\boldsymbol{D_R}$ of index two of the representative space group $\boldsymbol{F}$. In the first column, we give the sequential number and symbol of the space-group type *F*. In the second column are listed subgroups $\boldsymbol{D_R}$ of index two of the representative space group $\boldsymbol{F}$ in the notation, using Opechowski & Guccione's (1965) conventions, based on the use of *ITC*52. Subgroups $\boldsymbol{D_R}$ belonging to the same space-group type are listed together. In the third column, the symbol of that space-group type is given. In the last column is a list of the same subgroups in the notation, using Opechowski & Gucciones's (1965) conventions, based on the use of *ITC*83. Symbols on the same line in columns two and four are the *ITC*52- and *ITC*83-based symbols of the same subgroup.

For example, for the space-group type No. 45, whose symbol is $F = Iba2$, there are four subgroups $\boldsymbol{D_R}$ of the representative space group $\boldsymbol{F} = \boldsymbol{Iba2}$ belonging to three types of space groups. The symbol, for example, of the subgroup of type *Pcc*2 is, using *ITC*52, $\boldsymbol{I_Pba2}$, while it is, using *ITC*83, $\boldsymbol{I_Pb'a'2}$. For space group No. 206, *Ia*3, we give in parentheses the notation where 3 is replaced with $\bar{3}$, see §4.

4. Other changes in space-group symbols and their impact on OG symbols

In *ITC*83, new symbols were introduced for the space-group types numbered 200–206 and 221–230. The Hermann–Mauguin symbols for these cubic space-group types belonging to the two cubic crystal classes $m\bar{3}$ and $m\bar{3}m$ now contain the symbol $\bar{3}$ instead of 3. Changes in the OG symbols due to these changes in cubic space-group-type symbols are: If in the OG symbol (based on *ITC*52) an unprimed (primed) letter is to the left of 3, it is replaced by an unprimed (primed) $\bar{3}$, *e.g.* $\boldsymbol{Im3}$ and $\boldsymbol{Ia'3}$ become $\boldsymbol{Im\bar{3}}$ and $\boldsymbol{Ia'\bar{3}'}$, respectively. There are two exceptions, the symbols $\boldsymbol{I_Pa3}$ and $\boldsymbol{I_Pa'3}$ become $\boldsymbol{I_Pa\bar{3}'}$ and $\boldsymbol{I_Pa'\bar{3}}$, respectively. If one interprets the OG symbols using *ITC*83, then one uses the same rule as above with no exceptions.†

In the most recent edition of *International Tables for Crystallography* (1995) [Section 1.3 of the Fourth,

Table 2. *Subgroups $\boldsymbol{D_R}$ of $\boldsymbol{F}$ for space-group types F where the differences in the printed coordinate triplets of general positions in ITC52 and ITC83 result in different OG symbols*

F	*ITC*52	$\boldsymbol{D_R}$ type	*ITC*83
No. 45 *Iba*2	$\boldsymbol{I_Pba2}$	*Pcc*2	$\boldsymbol{I_Pb'a'2}$
	$\boldsymbol{I_Pba'2'}$	$Pca2_1$	$\boldsymbol{I_Pb'a2'}$
	$\boldsymbol{I_Pb'a2'}$		$\boldsymbol{I_Pba'2'}$
	$\boldsymbol{I_Pb'a'2}$	*Pba*2	$\boldsymbol{I_Pba2}$
No. 67 *Cmma*	$\boldsymbol{C_Pmma}$	*Pccm*	$\boldsymbol{C_Pmm'a'}$
	$\boldsymbol{C_Pm'm'a'}$		$\boldsymbol{C_Pm'ma}$
	$\boldsymbol{C_Pm'ma}$	*Pcca*	$\boldsymbol{C_Pm'm'a'}$
	$\boldsymbol{C_Pm'ma'}$		$\boldsymbol{C_Pm'm'a}$
	$\boldsymbol{C_Pmm'a}$	*Pmma*	$\boldsymbol{C_Pmma'}$
	$\boldsymbol{C_Pmm'a'}$		$\boldsymbol{C_Pmma}$
	$\boldsymbol{C_Pmma'}$	*Pbcm*	$\boldsymbol{C_Pmm'a}$
	$\boldsymbol{C_Pm'm'a}$		$\boldsymbol{C_Pm'ma'}$
	$\boldsymbol{C_Imma}$	*Ibam*	$\boldsymbol{C_Imm'a'}$
	$\boldsymbol{C_Imma'}$		$\boldsymbol{C_Imm'a}$
	$\boldsymbol{C_Im'm'a}$		$\boldsymbol{C_Im'ma'}$
	$\boldsymbol{C_Im'm'a'}$		$\boldsymbol{C_Im'ma}$
	$\boldsymbol{C_Imm'a}$	*Imma*	$\boldsymbol{C_Imma'}$
	$\boldsymbol{C_Imm'a'}$		$\boldsymbol{C_Imma}$
	$\boldsymbol{C_Im'ma'}$	*Ibca*	$\boldsymbol{C_Im'm'a}$
	$\boldsymbol{C_Im'ma}$		$\boldsymbol{C_Im'm'a'}$
No. 68 *Ccca*	$\boldsymbol{C_Pcca}$	*Pban*	$\boldsymbol{C_Pc'ca'}$
	$\boldsymbol{C_Pc'c'a'}$		$\boldsymbol{C_Pcc'a}$
	$\boldsymbol{C_Pc'ca}$	*Pcca*	$\boldsymbol{C_Pcca'}$
	$\boldsymbol{C_Pc'ca'}$		$\boldsymbol{C_Pcca}$
	$\boldsymbol{C_Pcca'}$	*Pbcn*	$\boldsymbol{C_Pc'ca}$
	$\boldsymbol{C_Pc'c'a}$		$\boldsymbol{C_Pcc'a'}$
	$\boldsymbol{C_Pcc'a'}$	*Pnna*	$\boldsymbol{C_Pc'c'a}$
	$\boldsymbol{C_Pcc'a}$		$\boldsymbol{C_Pc'c'a'}$
No. 72 *Ibam*	$\boldsymbol{I_pbam}$	*Pccm*	$\boldsymbol{I_pb'a'm}$
	$\boldsymbol{I_pb'am}$	*Pbcm*	$\boldsymbol{I_pba'm}$
	$\boldsymbol{I_pba'm}$		$\boldsymbol{I_pb'am}$
	$\boldsymbol{I_pbam'}$	*Pccn*	$\boldsymbol{I_pb'a'm'}$
	$\boldsymbol{I_pb'a'm}$	*Pbam*	$\boldsymbol{I_pbam}$
	$\boldsymbol{I_pb'am'}$	*Pbcn*	$\boldsymbol{I_pba'm'}$
	$\boldsymbol{I_pba'm'}$		$\boldsymbol{I_pb'am'}$
	$\boldsymbol{I_pb'a'm'}$	*Pban*	$\boldsymbol{I_pbam'}$
No. 73 *Ibca*	$\boldsymbol{I_pbca}$	*Pbca*	$\boldsymbol{I_pb'c'a'}$
	$\boldsymbol{I_pb'c'a'}$		$\boldsymbol{I_pbca}$
	$\boldsymbol{I_pb'ca}$	*Pcca*	$\boldsymbol{I_pbc'a'}$
	$\boldsymbol{I_pbc'a}$		$\boldsymbol{I_pb'ca'}$
	$\boldsymbol{I_pbca'}$		$\boldsymbol{I_pb'c'a}$
	$\boldsymbol{I_pbc'a'}$		$\boldsymbol{I_pb'ca}$
	$\boldsymbol{I_pb'ca'}$		$\boldsymbol{I_pbc'a}$
	$\boldsymbol{I_pb'c'a}$		$\boldsymbol{I_pbca'}$
No. 108 *I*4*cm*	$\boldsymbol{I_PAcm}$	*P*4*bm*	$\boldsymbol{I_PAc'm'}$
	$\boldsymbol{I_PA'c'm}$	$P4_2cm$	$\boldsymbol{I_PA'cm'}$
	$\boldsymbol{I_PA'cm'}$	$P4_2bc$	$\boldsymbol{I_PA'c'm}$
	$\boldsymbol{I_PAc'm'}$	*P*4*cc*	$\boldsymbol{I_PAcm}$
No. 206 *Ia*3	$\boldsymbol{I_Pa3}$ ($\boldsymbol{I_Pa\bar{3}'}$)	$Pa\bar{3}$	$\boldsymbol{I_Pa'3}$ ($\boldsymbol{I_Pa'\bar{3}'}$)
	$\boldsymbol{I_Pa'3}$ ($\boldsymbol{I_Pa'\bar{3}}$)		$\boldsymbol{I_Pa3}$ ($\boldsymbol{I_Pa\bar{3}}$)
No. 214 $I4_132$	$\boldsymbol{I_PA_132}$	$P4_332$	$\boldsymbol{I_PA_1'32'}$
	$\boldsymbol{I_PA_1'32'}$	$P4_132$	$\boldsymbol{I_PA_132}$

† The author would like to thank a referee for pointing out this simple rule when changing the notation from 3 to $\bar{3}$.

revised edition (*ITC*95)], the symbol *e* has been introduced for double glide planes. As a consequence, the Hermann–Mauguin symbol of five space-group types have been given a second symbol containing this symbol *e*: No. 39 *Abm*2/*Aem*2, No. 41 *Aba*2/*Aea*2, No. 64 *Cmca*/*Cmce*, No. 67 *Cmma*/*Cmme* and No. 68 *Ccca*/*Ccce*.

Using the conventions of §2, the representative space group ***Abm*2** has the translation subgroup

$$\mathbf{A} = \langle (1|0\tfrac{1}{2}\tfrac{1}{2}), (1|0\tfrac{1}{2}\bar{\tfrac{1}{2}}), (1|100)\rangle$$

and the set of coset representatives of ***Abm*2** with respect to $\mathbf{A}$ are:

$$(1|000), \quad (2_z|000), \quad (m_y|0\tfrac{1}{2}0), \quad (m_x|0\tfrac{1}{2}0). \qquad (5)$$

The group ***Abm*2** contains both the elements $(m_x|0\tfrac{1}{2}0)$ and $(m_x|00\tfrac{1}{2})$, the double glide plane, *i.e.* both a $b(\tfrac{1}{4}, y, z)$ glide plane and a $c(\tfrac{1}{4}, y, z)$ glide plane. However, the symbol for this space group contains only the symbol *b*. Consequently, it was decided to replace *b* by the letter *e*, which would represent both the *b* and *c* glide planes of this double glide plane. We choose not to use this new notation in symbols for magnetic groups.

The reason for this is as follows: For example, the subgroup $\mathbf{D_R} = \mathbf{A_P b'm'2}$ of ***Abm*2** is defined, using the conventions of §2, by the translational subgroup

$$\mathbf{A_P} = \langle (1|100), (1|010), (1|001)\rangle$$

and the coset representatives

$$(1|000), (2_z|000), (m_y|00\tfrac{1}{2}), (m_x|00\tfrac{1}{2}),$$

where the coset representatives $(m_y|0\tfrac{1}{2}0)$ and $(m_x|0\tfrac{1}{2}0)$ of (5) have been multiplied by $t_\alpha = (1|0\tfrac{1}{2}\tfrac{1}{2})$. This implies that the magnetic space group $\mathbf{A_P b'm'2}$ contains the operations $(m_x|00\tfrac{1}{2})$ and $(m_x|0\tfrac{1}{2}0)'$. That is, in this magnetic space group, the *b* glide plane implied by $(m_x|0\tfrac{1}{2}0)$ is primed, *i.e.* coupled with time inversion, while the *c* glide plane implied by $(m_x|00\tfrac{1}{2})$ is not. By meticulously following the Opechowski–Guccione convention given in §2, there is no ambiguity when replacing the symbol $\mathbf{A_P b'm'2}$ by $\mathbf{A_P e'm'2}$. However, since the symbol *e* is associated with both glide planes, the use of a magnetic space-group-type symbol incorporating *e* when only one of the two glide planes is primed could be confusing.

This work is dedicated to the memory of Professor W. Opechowski, my scientific 'father'. I thank Professor H. Wondratschek for reading and commenting on an earlier version of this paper. This work was supported by the National Science Foundation under grant DMR-9510335.

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