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CHANGES IN THE OPECHOWSKI-GUCCIONE SYMBOLS FOR MAGNETIC SPACE GROUPS DUE TO CHANGES IN THE INTERNATIONAL TABLES OF CRYSTALLOGRAPHY

D. B. LITVIN

Department of Physics, The Pennsylvania State University, Penn State-Berks Campus, P.O. Box 7009, Reading, PA 196106009, U.S.A

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The conventions given for interpreting the Opechowski-Guccione symbols for magnetic space group depend in part on the printed coordinate triplets of general positions given in the International Tables of Crystallography. Changes have been made in these printed coordinate triplets for some centered space groups. Consequently, to avoid ambiguities, the symbol for some magnetic group types are changed.

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Opechowski and Guccione (1965) (see also Opechowski, (1986) and Opechowski and Litvin (1977)) give a list of symbols for the 1191 types of magnetic space groups. Each symbol is as symbol for a *representative* magnetic space M group belonging to that type. To uniquely define each symbol a uniquely defined symbol for one *representative* space group F from each of the 230 types of space groups was required. The symbol for and definition of each representative space group is as follows:

In the *International Tables For X-ray Crystallography*, Volume 1 (1952) (abbreviated by ITC52), which was used by Opechowski and Guccione, one finds at the top of the first page of tabulations for a space group type a symbol for that space group type. This is taken as the symbol of the representative space group of that type. A specification of the coordinate system used is given and in terms of that coordinate system a specification of the subgroup T of translations of the representative space group. The space

group F is defined by the translation subgroup T and a set of n coset representatives of T in F. These coset representatives are indirectly specified by the printed set of coordinate triplets of the exactly n general positions.

For example, consider the space group type Number 72, Ibam (page 164 of ITC52 (third edition (1969)). Translational subgroup is

$$\mathrm{I} = \langle (1|1\ 0\ 0),\quad (1|0\ 1\ 0),\quad (1|1/2\ 1/2\ 1/2)\rangle$$

and the coordinate triplets of the general positions printed on page 164 are :

$$\begin{array}{llll} x,y,z; & \bar{x},\bar{y},z & \bar{x},y,\bar{z}+1/2 & x,\bar{y},\bar{z}+1/2 \\ \bar{x},\bar{y},\bar{z} & x,y,\bar{z} & x,\bar{y},z+1/2 & \bar{x},y,z+1/2 \end{array}$$

Consequently, the coset representatives of the translation subgroup $T=I$ in the representative space group $F=$ Ibam are:

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

The translation subgroup $T=$ I and this set of coset representatives uniquely defines the representative space group $F=$ Ibam.

The changes required in symbols of magnetic space groups are only among the magnetic space groups M_R, those with a translation subgroup with one half of the translations primed, i.e., coupled with time inversion. A magnetic space group M_R that belongs to the family of a space group F has the form $M_R = D_R + (F-D_R)1'$, where D_R is an equi-class subgroup of index 2 in F, and $1'$ is time inversion. A symbol given by Opechowski and Guccione specifies both D_R and F and consequently is used as a symbol of the corresponding magnetic space group M_R.

The magnetic space group M_R is defined as follows by defining a subgroup D_R in F: For a given representative space group F one selects on of the subgroups $T^D$of index 2 in T. One also selects one translation t_α which belongs to T but not to T^D. The subgroup D_R is specified by a set of coset representatives of T^D in D_R. This set of coset representatives is obtained from the set of coset representatives of T in F (implied by the set of coordinate triplets of the general positions printed in ITC52) by multiplying by t_α some, or possibly none, of the coset representatives.

The symbol for D_R of F is assigned by taking the symbol for F and then replacing the symbol for T by a symbol for the translation subgroup $T^D$of D_R. Also, each letter or numeral in the symbol of F is primed if the

associated coset representative has been multiplied by t_α. For example consider $F=$ Ibam. A subgroup D_R is defined by the translation subgroup $T^D = \mathrm{I_P}$ of $T=\mathrm{I}$

$$\mathrm{I_P} = \langle (1|1\ 0\ 0), \quad (1|0\ 1\ 0), \quad (1|0\ 0\ 1) \rangle$$

and the coset representatives given in Eq. (1). We have $D_R = \mathrm{I_P bam}$, which is also the symbol for the magnetic space group $M_R = \mathrm{I_P bam}$. If one instead would take the coset representatives as

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

then one has the group $D_R = \mathrm{I_P b'a'm}$.

ITC52 has been replaced with the *International Tables for Crystallography*, Volume A (1983) (abbreviated by ITC83). In ITC83, for some space groups, the explicitly printed coordinate triplets of general positions differ from that printed in ITC52. Using the conventions of Opechowski and Guccione and ITC83 leads to differing symbols for the same magnetic space groups. For example, using ITC83 one finds for the space group $F=$ Ibam (page 317 of the fourth edition of ITC83 (1995)) the same translation subgroup $T=\mathrm{I}$. However, the coset representatives implied by the printed coordinate triplets of the general positions are those given in Eq. (2) and not those given in Eq. (1), i.e., not those found by using ITC52. Consequently one finds that for the two magnetic space groups derived above using ITC52 their symbols change when using ITC83:

$$\begin{aligned} \mathrm{I_P b'a'm\ (ITC52)} &\equiv \mathrm{I_P bam\ (ITC83)} \\ \mathrm{I_P bam\ (ITC52)} &= \mathrm{I_P b'a'm\ (ITC83)} \end{aligned}$$

In Table I we give the changes in the Opechowski-Guccione symbols for magnetic space group types required if one used ITC83.

A more detailed analysis, including the relationship to the Belov, Neronova, Smirnova (1957) symbols for magnetic space groups, and additional changes to due to the change in the notation for the two cubic crystal classes $m3$ and $m3m$ which now contain the symbol 3 instead of 3, and the introduction of the symbol "e" into the symbols for space groups is given elsewhere (Litvin (1997)).

TABLE I Changes in Opechowski-Guccione symbols of magnetic space group types due to changes in the printed coordinate triplets of general positions from ITC52 to ITC83

F	*ITC52*	*ITC83*
#45 Iba2	I_Pba2	$I_Pb'a'2$
	$I_Pba'2'$	$I_Pb'a2'$
	$I_Pb'a'2$	I_Pba2
#67 Cmma	C_Pmma	$C_Pm'ma$
	$C_Pm'ma$	$C_Pm'm'a'$
	$C_Pmm'a$	C_Pmma
	C_Pmma'	$C_Pmm'a$
	C_Imma	$C_Pm'ma$
	$C_Imm'a$	C_Imma
	$C_Im'ma'$	$C_Im'm'a'$
#68 Ccca	C_Pcca	$C_Pcc'a$
	$C_Pc'ca$	C_Pcca
	C_Pcca'	$C_Pc'ca$
	$C_Pcc'a'$	$C_Pc'c'a'$
#72 Ibam	I_Pbam	$I_Pb'a'm$
	$I_Pb'am$	$I_Pb'am$
	I_Pbam'	$I_Pb'a'm'$
	$I_Pb'a'm$	I_Pbam
	$I_Pb'am'$	$I_Pba'm'$
	$I_Pb'a'm'$	I_Pbam'
#98 $I4_122$	I_P4_122	I_P4_122
	$I_P4_1'22'$	$I_P4_1'22'$
	$I_P4_12'2'$	$I_P4_12'2'$
	$I_P4_1'2'2$	$I_P4_1'2'2$
#108 I4cm	I_P4cm	$I_P4c'm'$
	$I_P4'c'm$	$I_P4'cm'$
	$I_P4'cm'$	$I_P4'c'm$
	$I_P4c'm'$	I_P4cm
#214 $I4_132$	I_P4_132	$I_P4_1'32'$
	$I_P4_1'32'$	I_P4_132

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