Acta Cryst. (1977). A**33**, 985–986

Subgroups and Changes of Standard Setting of Triclinic and Monoclinic Space Groups

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(*Received* 17 *January* 1977; *accepted* 1 *June* 1977)

The paper gives the first *complete* list of subgroups and changes of standard setting for every triclinic and monoclinic space group. The method determines the conditions that the standard setting of a group g must fulfil, with respect to the standard setting of a group G, so that the generators of g belong to G.

A few years ago, a new interest was taken in the study of subgroups (which are again space groups) of space groups and especially the study of maximal subgroups. There are two categories of maximal subgroups: subgroups having the same translation lattice (*translationengleich*) and subgroups belonging to the same crystal class (*klassengleich*) as the space group. Nonmaximal subgroups are infinite in number whereas *translationengleich* maximal subgroups are finite in number; on the other hand *klassengleich* maximal subgroups whose standard symbol is distinct from the space-group standard symbol are also finite in number (Neubuser & Wondratschek, 1966*a*, *b*), whereas maximal subgroups whose standard symbol is the same as for the space group (isosymbolic subgroups) may be infinite in number. These are the reasons why most papers have essentially been devoted to nonisosymbolic maximal subgroups (Neubuser & Wondratschek, 1966*a*, *b*; Boyle & Lawrenson, 1972*a*, *b*; Bertaut, 1976*a*, *b*). One of us (Billiet, 1973), using a different method, derived all isosymbolic, maximal and nonmaximal, subgroups from every space group; this method has been extended to other types of maximal and nonmaximal subgroups (Billiet, Sayari & Zarrouk, 1977), making possible the systematic derivation of all the subgroups of every space group. The method determines the conditions that the standard setting (o,a,b,c) of a group g must fulfil, with reference to the standard setting (O,A,B,C) of a group G, so that the generators of g do belong to G, *i.e.*, g *is indeed* a subgroup of G; thus the coordinates (X_o, Y_o, Z_o) of the origin o of the g setting, with reference to (O,A,B,C), are found likewise to be the coefficients of the square matrix S of the transformation from the vectors (A,B,C) to the vectors (a,b,c), *i.e.* $(a,b,c)=(A,B,C)S$; the matrix determinant, Det S, is necessarily positive because standard settings are right-handed. Therefore *every* standard setting of *absolutely any* subgroup – maximal or nonmaximal, *translationengleich*, *klassengleich*, isosymbolic or not – of *every* space group can be obtained. If the standard symbol of g is the same as for G and if Det $S=1$, then g is identical to G and (o,a,b,c) is another standard setting of G. Therefore the method also allows the

Table 1. *Transformation matrices for triclinic and monoclinic space groups*

For all the monoclinic space groups and subgroups the available standard setting is the 'first setting'.

Triclinic

$$T=\begin{vmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{vmatrix};$$

T_1: all coefficients are integers; Det $T_1 \geq 1$.
T_2: $2m_{11}$ and $2m_{31}$ are both even or odd integers; $2m_{12}$ and $2m_{32}$ are both even or odd integers; $2m_{13}$ and $2m_{33}$ are both even or odd integers; m_{21}, m_{22} and m_{23} are integers; Det $T_2 \geq \frac{1}{2}$.

Monoclinic

$$M=\begin{vmatrix} m_{11} & m_{12} & 0 \\ m_{21} & m_{22} & 0 \\ 0 & 0 & m_{33} \end{vmatrix};$$ $m_{11}, m_{12}, m_{21}, m_{22}$ and m_{33} are integers in all the following matrices.

M_1 : no special values; Det $M_1 \geq 1$.
M_2 : m_{33} is odd; Det $M_2 \geq 1$.
M_3 : m_{33} is even; Det $M_3 \geq 2$.
M_4 : m_{12} and m_{22} are odd; Det $M_4 \geq 1$.
M_5 : m_{12} is even; m_{22} is odd; Det $M_5 \geq 1$.
M_6 : m_{12} is odd; m_{22} is even; Det $M_6 \geq 1$.
M_7 : m_{12} and m_{22} are even; Det $M_7 \geq 2$.
M_8 : m_{12}, m_{22} and m_{33} are odd; Det $M_8 \geq 1$.
M_9 : m_{12} is even; m_{22} and m_{33} are odd; Det $M_9 \geq 1$.
M_{10}: m_{12} and m_{33} are odd; m_{22} is even; Det $M_{10} \geq 1$.
M_{11}: m_{12} and m_{22} are even; m_{33} is odd; Det $M_{11} \geq 2$.
M_{12}: m_{12} and m_{22} are odd; m_{33} is even; Det $M_{12} \geq 2$.
M_{13}: m_{12} and m_{33} are even; m_{22} is odd; Det $M_{13} \geq 2$.
M_{14}: m_{12} is odd; m_{22} and m_{33} are even; Det $M_{14} \geq 2$.
M_{15}: m_{12}, m_{22} and m_{33} are even; Det $M_{15} \geq 4$.
M_{16}: m_{11} and m_{33} are both even or odd; m_{21} is even; Det $M_{16} \geq 1$.
M_{17}: m_{11} and m_{33} are both even or odd; m_{12} and m_{22} are odd; m_{21} is even; Det $M_{17} \geq 1$.
M_{18}: m_{11} and m_{33} are both even or odd; m_{12} and m_{21} are even; m_{22} is odd; Det $M_{18} \geq 1$.
M_{19}: m_{11} and m_{33} are both even or odd; m_{12} is odd; m_{21} and m_{22} are even; Det $M_{19} \geq 2$.
M_{20}: m_{11} and m_{33} are both even or odd; m_{12}, m_{21} and m_{22} are even; Det $M_{20} \geq 2$.
M_{21}: m_{11}, m_{21} and m_{33} are even; Det $M_{21} \geq 4$.
M_{22}: m_{11}, m_{12}, m_{21} and m_{33} are even; m_{22} is odd; Det $M_{22} \geq 4$.
M_{23}: m_{11}, m_{12}, m_{21}, m_{22} and m_{33} are even; Det $M_{23} \geq 8$.

determination of all the changes of standard setting of the space groups (Zarrouk & Billiet, 1975; Zarrouk, 1976; Billiet, Sayari & Zarrouk, 1977). As a result, one can also characterize the collection of settings which are relevant to a given subgroup g_i of space group G. Numerous details about this derivation can be found elsewhere (Billiet, 1973; Sayari & Billiet, 1975; Sayari, 1976; Billiet, Sayari & Zarrouk, 1977).

The aim of the present paper is to illustrate the efficiency of the method by listing *completely* the subgroups and the changes of standard setting of the triclinic and monoclinic space groups. Transformation matrices are given in Table 1; coordinates of permissible origins are given in Table 2. In Table 3, appropriate matrices (from Table 1) and origins (from Table 2) are chosen for every subgroup and change of standard setting for each triclinic and monoclinic space group. Proofs of the completeness of the tables can be found in other papers (Billiet, 1973; Billiet, Sayari & Zarrouk, 1977). Analogous tables are under preparation for other crystal systems. We have not noted any substantial dissension with other partial results from the literature.

In conclusion, we remark that several previous works have been devoted to the determination of maximal subgroups; their purpose is attractive: by iteration of their method one can get sequences of maximal subgroups and eventually determine all the subgroups of a given space group; but our own experience has pointed out that the direct derivation of all the subgroups is very easy compared to the specific derivation of maximal subgroups; this may appear surprising. As a matter of fact, the investigation of the maximal subgroups is a *very interesting and difficult mathematical problem*, particularly the investigation of the isosymbolic maximal subgroups of space groups such as $P1$, $P2$, $P3$, $P4$, $P6$ *etc.* (Sayari, 1976). We think, having ourselves succumbed to it, that the endeavour to specifically derive maximal subgroups has slowed down the resolution of the *fundamental crystallographic problem*: the determination of all subgroups of a space group.

Table 2. *Coordinates of permissible origins*

X_o, Y_o, Z_o: the coordinates of the origin o are real numbers in all the following cases.
o_1: no special values.
o_2: $2Z_o$ is any integer.
o_3: $4Z_o$ is any odd integer.
o_4: $2X_o$ and $2Y_o$ are integers.
o_5: $4X_o$ is any odd integer; $2Y_o$ is any integer.
o_6: $2X_o$ is any integer; $4Y_o$ is any odd integer.
o_7: $4X_o$ and $4Y_o$ are odd integers.
o_8: $2X_o$, $2Y_o$ and $2Z_o$ are integers.
o_9: $4X_o$ and $4Z_o$ are odd integers; $2Y_o$ is any integer.

Table 3. *Appropriate matrices and origins for every subgroup and change of standard setting for all triclinic and monoclinic space groups*

Space group	
$P1$	$P1^*$: (T_1,o_1)
$P\bar{1}$	$P1$: (T_1,o_1); $P\bar{1}^*$: (T_1,o_8)
$P2$	$P1$: (T_1,o_1); $P2^*$: (M_1,o_4); $P2_1$: (M_3,o_4); $B2$: (M_{21},o_4)
$P2_1$	$P1$: (T_1,o_1); $P2_1^*$: (M_2,o_4)
$B2$	$P1$: (T_2,o_1); $P2$: (M_1,o_4); $P2_1$: (M_2,o_5), (M_3,o_4); $B2^*$: (M_{16},o_4)
Pm	$P1$: (T_1,o_1); Pm^*: (M_1,o_2); Pb: (M_7,o_2); Bm: (M_{21},o_2); Bb: (M_{23},o_2)
Pb	$P1$: (T_1,o_1); Pb^*: (M_5,o_2); Bb: (M_{22},o_2)
Bm	$P1$: (T_2,o_1); Pm: (M_1,o_2); Pb: (M_6,o_3), (M_7,o_2); Bm^*: (M_{16},o_2); Bb: (M_{19},o_3), (M_{20},o_2)
Bb	$P1$: (T_2,o_1); Pb: (M_4,o_3), (M_5,o_2); Bb^*: (M_{17},o_3), (M_{18},o_2)
$P2/m$	$P1$: (T_1,o_1); $P\bar{1}$: (T_1,o_8); $P2$: (M_1,o_4); $P2_1$: (M_3,o_4); $B2$: (M_{21},o_4); Pm: (M_1,o_2); Pb: (M_7,o_2); Bm: (M_{21},o_2); Bb: (M_{23},o_2); $P2/m^*$: (M_1,o_8); $P2_1/m$: (M_3,o_8); $B2/m$: (M_{21},o_8); $P2/b$: (M_7,o_8); $P2_1/b$: (M_{15},o_8); $B2/b$: (M_{23},o_8)
$P2_1/m$	$P1$: (T_1,o_1); $P\bar{1}$: (T_1,o_8); $P2_1$: (M_2,o_4); Pm: (M_1,o_3); Pb: (M_7,o_3); Bm: (M_{21},o_3); Bb: (M_{23},o_3); $P2_1/m^*$: (M_2,o_8); $P2_1/b$: (M_{11},o_8)
$B2/m$	$P1$: (T_2,o_1); $P\bar{1}$: (T_2,o_8), (T_2,o_9); $P2$: (M_1,o_4); $P2_1$: (M_2,o_5), (M_3,o_4); $B2$: (M_{16},o_4); Pm: (M_1,o_2); Pb: (M_6,o_3), (M_7,o_2); Bm: (M_{16},o_2); Bb: (M_{19},o_3), (M_{20},o_2); $P2/m$: (M_1,o_8); $P2_1/m$: (M_2,o_9), (M_3,o_8); $B2/m^*$: (M_{16},o_8); $P2/b$: (M_6,o_9), (M_7,o_8); $P2_1/b$: (M_{10},o_8), (M_{11},o_9), (M_{14},o_9), (M_{15},o_8); $B2/b$: (M_{19},o_9), (M_{20},o_8)
$P2/b$	$P1$: (T_1,o_1); $P\bar{1}$: (T_1,o_8); $P2$: (M_1,o_6); $P2_1$: (M_3,o_6); $B2$: (M_{21},o_6); Pb: (M_5,o_2); Bb: (M_{22},o_2); $P2/b^*$: (M_5,o_8); $P2_1/b$: (M_{13},o_8); $B2/b$: (M_{22},o_8)
$P2_1/b$	$P1$: (T_1,o_1); $P\bar{1}$: (T_1,o_8); $P2_1$: (M_2,o_6); Pb: (M_5,o_3); Bb: (M_{22},o_3); $P2_1/b^*$: (M_9,o_8)
$B2/b$	$P1$: (T_2,o_1); $P\bar{1}$: (T_2,o_8), (T_2,o_9); $P2$: (M_1,o_6); $P2_1$: (M_2,o_7), (M_3,o_6); $B2$: (M_{16},o_6); Pb: (M_4,o_3), (M_5,o_2); Bb: (M_{17},o_3), (M_{18},o_2); $P2/b$: (M_4,o_9), (M_5,o_8); $P2_1/b$: (M_8,o_8), (M_9,o_9), (M_{12},o_9), (M_{13},o_8); $B2/b^*$: (M_{17},o_9), (M_{18},o_8)

* Change in standard setting if Det $S=1$; isosymbolic subgroup if Det $S>1$.

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