

Table 1. Time ratios for the triangular peak

$(B - A)/A$	$T_{c.t.}/T_{abs.}$	$T_{c.c.}/T_{abs.}$
0	1	1
1	1.005	1.05
10	1.05	1.60
100	1.10	3.07
1000	1.12	4.92
∞	1.125	$\infty \left(= 0.75 \ln \frac{B - A}{A} \right)$

(2) *Calculations required.* In this respect the constant-time method is the best, as only the intensity integrals appear, which must be calculated anyway for finding I . Next is the absolute optimization, where in each range one integral, that of \sqrt{Y} , is needed. The worst is the constant-count method, where in each range two integrals, those of Y^2 and of $1/Y$, must be calculated.

(3) *Experimental feasibility.* We have also to keep in mind that the constant-time and the constant-count methods are equally easy to perform, whereas the measurements corresponding to the absolute optimization would be rather laborious.

4. Conclusions

The constant-time should always be preferred to the constant-count method, as the latter is in no respect better than the former. The selection between the constant time and the absolute methods is somewhat arbitrary, as in some respects one or the other is favoured. For most practical cases, however, we would use the constant-time method.

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Complete List of Subgroups and Changes of Standard Setting of Two-Dimensional Space Groups

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To illustrate the efficiency of a systematic method of derivation of subgroups [Billiet, *Bull. Soc. Fr. Minéral. Cristallogr.* (1973), **96**, 327–334], the authors have tabulated the complete list of standard settings of every subgroup of any two-dimensional space group.

In other papers (Billiet, 1973; Billiet, Sayari & Zarrouk, 1978), we have given much information, concerning a systematic method of deriving subgroups (which are

space groups again) of space groups. This method has enabled us to find all the subgroups of the triclinic and monoclinic space groups (Sayari & Billiet, 1977).

Here a new example of the efficiency of this method is given. We have listed the subgroups and the changes of standard setting of the two-dimensional space

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Table 1. *Forms and coefficient values of the transformation matrices*

Type M

$$M = \begin{vmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{vmatrix}$$

M_1 : all coefficients are integers; $\det M_1 \geq 1$

M_2 : $n_{11} = n_{22}$ = any integer; $n_{21} = -n_{12}$ = any integer; $\det M_2 \geq 1$

M_3 : $n_{11} = n_{21} = n_{22} = -n_{12}$ = any integer; $\det M_3 \geq 2$

M_4 : $n_{11} = n_{12} = n_{22} = -n_{21}$ = any integer; $\det M_4 \geq 2$

M_5 : $2n_{11}$ and $2n_{21}$ are both even or odd; $2n_{12}$ and $2n_{22}$ are both even or odd; $\det M_5 \geq \frac{1}{2}$

Type Nⁱ

$$N^1 = \begin{vmatrix} n_1 & 0 \\ 0 & n_2 \end{vmatrix}; N^2 = \begin{vmatrix} 0 & -n_2 \\ n_1 & 0 \end{vmatrix};$$

n_1 and n_2 are integers for all the following matrices

N_1^i : no special values; $\det N_1^i \geq 1$

N_2^i : n_1 is even; $\det N_2^i \geq 2$

N_3^i : n_1 is odd; $\det N_3^i \geq 1$

N_4^i : n_2 is even; $\det N_4^i \geq 2$

N_5^i : n_2 is odd; $\det N_5^i \geq 1$

N_6^i : n_1 and n_2 are even; $\det N_6^i \geq 4$

N_7^i : n_1 and n_2 are odd; $\det N_7^i \geq 1$

N_8^i : n_1 is even; n_2 is odd; $\det N_8^i \geq 2$

N_9^i : n_1 is odd; n_2 is even; $\det N_9^i \geq 2$

N_{10}^i : $n_1 = n_2$; $\det N_{10}^i \geq 1$

N_{11}^i : $n_1 = n_2$ = any even integer; $\det N_{11}^i \geq 4$

N_{12}^i : $n_1 = n_2$ = any odd integer; $\det N_{12}^i \geq 1$

Type Pⁱ

$$P^1 = \begin{vmatrix} n_1 & -n_2 \\ n_1 & n_2 \end{vmatrix}; \quad P^2 = \begin{vmatrix} n_1 & n_2 \\ -n_1 & n_2 \end{vmatrix}; \quad P^3 = \begin{vmatrix} n_1 & n_2 \\ 0 & 2n_2 \end{vmatrix};$$

$$P^4 = \begin{vmatrix} 0 & 2n_2 \\ n_1 & n_2 \end{vmatrix}; \quad P^5 = \begin{vmatrix} n_1 & n_2 \\ 2n_1 & 0 \end{vmatrix}; \quad P^6 = \begin{vmatrix} 2n_1 & 0 \\ n_1 & n_2 \end{vmatrix};$$

n_1 and n_2 are integers for all the following matrices

P_1^i : no special values; $\det P_1^i \geq 2$

P_2^i : n_1 is even; $\det P_2^i \geq 4$

P_3^i : n_1 is odd; $\det P_3^i \geq 2$

P_4^i : n_2 is even; $\det P_4^i \geq 4$

P_5^i : n_2 is odd; $\det P_5^i \geq 2$

P_6^i : n_1 and n_2 are both even or odd; $\det P_6^i \geq 8$ or $\det P_6^i \geq 2$

P_7^i : n_1 and n_2 are not of the same parity; $\det P_7^i \geq 4$

Type Q

$$Q = \begin{vmatrix} n_1 & -n_2 \\ n_2 & n_1 - n_2 \end{vmatrix};$$

n_1 and n_2 are integers for all the following matrices

Q_1 : no special values; $\det Q_1 \geq 1$

Q_2 : $n_1 = n_2$; $\det Q_2 \geq 1$

Q_3 : $n_1 = 0$; $\det Q_3 \geq 1$

Q_4 : $n_1 = 2n_2$; $\det Q_4 \geq 3$

Q_5 : $n_1 = -n_2$; $\det Q_5 \geq 3$

Q_6 : $2n_1 = n_2$; $\det Q_6 \geq 3$

groups. As far as we know, it is the first time that this complete list has been tabulated [see, for instance, a partial list of two-dimensional subgroups in *International Tables for X-ray Crystallography* (1952)].

The method determines the conditions that the standard setting $(\mathbf{o}, \mathbf{a}, \mathbf{b})$ of a space group g must fulfil, with respect to the standard setting $(\mathbf{O}, \mathbf{A}, \mathbf{B})$ of a space group G , so that the generators of g do belong to G . In Table 1, the matrices S of the appropriate transformations from the vectors (\mathbf{A}, \mathbf{B}) to the vectors (\mathbf{a}, \mathbf{b}) , i.e. $(\mathbf{a}, \mathbf{b}) = (\mathbf{A}, \mathbf{B})S$, are given. The determinants of the matrices, $\det S$, are positive because the standard settings are right handed. The coordinates (X_o, Y_o) of the permissible origins \mathbf{o} , with reference to $(\mathbf{O}, \mathbf{A}, \mathbf{B})$, are given in Table 2. In Table 3, suitable matrices (from Table 1) and origins (from Table 2) are chosen for every subgroup (of any given standard symbol) of each two-dimensional space group. If g and G have the same standard symbol and if $\det S = 1$, g is identical to G and $(\mathbf{o}, \mathbf{a}, \mathbf{b})$ is another setting of G ; these changes of standard setting are infinite in number for each space group. As a result, one can characterize the infinite collection of the settings which are relevant to a given subgroup g_i of the space group G . Numerous details of this method of derivation, further remarks on the

Table 2. *Coordinates of appropriate origins*

X_o, Y_o : the coordinates of the origin \mathbf{o} are real numbers in all the following cases (\mathbf{o}_1 to \mathbf{o}_{24}).

\mathbf{o}_1 : no special values

\mathbf{o}_2 : $2X_o$ is any integer

\mathbf{o}_3 : $2X_o$ is any even integer

\mathbf{o}_4 : $2X_o$ is any odd integer

\mathbf{o}_5 : $4X_o$ is any odd integer

\mathbf{o}_6 : $2Y_o$ is any integer

\mathbf{o}_7 : $2Y_o$ is any even integer

\mathbf{o}_8 : $2Y_o$ is any odd integer

\mathbf{o}_9 : $4Y_o$ is any odd integer

\mathbf{o}_{10} : $2X_o$ and $2Y_o$ are integers

\mathbf{o}_{11} : $2X_o$ and $2Y_o$ are even integers

\mathbf{o}_{12} : $2X_o$ and $2Y_o$ are odd integers

\mathbf{o}_{13} : $2X_o$ is any even integer, $2Y_o$ is any odd integer

\mathbf{o}_{14} : $2X_o$ is any odd integer, $2Y_o$ is any even integer

\mathbf{o}_{15} : $4X_o$ and $4Y_o$ are odd integers

(k, n, n' : integers in all the following cases)

\mathbf{o}_{16} : $X_o = k/3 + n$, $Y_o = 2k/3 + n'$

\mathbf{o}_{17} : $Y_o = X_o + k$

\mathbf{o}_{18} : $Y_o = X_o + (2k + 1)/2$

\mathbf{o}_{19} : $Y_o = 2X_o + k$

\mathbf{o}_{20} : $Y_o = 2X_o + (2k + 1)/2$

\mathbf{o}_{21} : $X_o = 2Y_o + k$

\mathbf{o}_{22} : $X_o = 2Y_o + (2k + 1)/2$

\mathbf{o}_{23} : $Y_o = -X_o + k$

\mathbf{o}_{24} : $Y_o = -X_o + (2k + 1)/2$

Table 3. Subgroups of two-dimensional space groups

An asterisk denotes an isosymbolic subgroup if $\det S > 1$, or change in standard setting if $\det S = 1$.

properties of subgroups and proofs of the completeness of the tables can be found elsewhere (Billiet, 1973; Billiet, Sayari & Zarrouk, 1978; Sayari, 1976; Zarrouk, 1976). Similar tables are under preparation for orthorhombic, tetragonal, trigonal, hexagonal and cubic systems. We are now enlarging the scope of this method to the derivation of subgroups of two-coloured space groups (Belguith & Billiet, 1978). As for physical applications of the results of the present paper, phase transitions in thin films, chemistry of surfaces and transitions between distinct smectic forms of a given mesomorphic substance come to mind.

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