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13.1. Isomorphic subgroups

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13.1.1. Definitions

A subgroup $\mathcal{H}$ of a space group $\mathcal{G}$ is an *isomorphic subgroup* if $\mathcal{H}$ is of the same or the enantiomorphic space-group type as $\mathcal{G}$. Thus, isomorphic space groups are a special subset of *klassengleiche subgroups*. The *maximal isomorphic subgroups of lowest index* are listed under **IIc** in the space-group tables of this volume (Part 7) (*cf.* Section 2.2.15). Isomorphic subgroups can easily be recognized because the standard space-group symbols of $\mathcal{G}$ and $\mathcal{H}$ are the same [isosymbolic subgroups (Billiet, 1973)] or the symbol of $\mathcal{H}$ is enantiomorphic to that of $\mathcal{G}$. Every space group has an infinite number of maximal isomorphic subgroups, whereas the number of maximal non-isomorphic subgroups is finite (*cf.* Section 8.3.3). For this reason, isomorphic subgroups are discussed in more detail in the present section.

If **a**, **b**, **c** are the basis vectors defining the conventional unit cell of $\mathcal{G}$ and $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ the basis vectors corresponding to $\mathcal{H}$ the relation

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{S} \qquad (13.1.1.1)$$

holds, where $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ and $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$ are row matrices and $\boldsymbol{S}$ is a (3×3) matrix. The coefficients S_{ij} of $\boldsymbol{S}$ are integers.*

The index of $\mathcal{H}$ in $\mathcal{G}$ is equal to $|\det(\boldsymbol{S})|$*, which is the ratio of the volumes $[\mathbf{a}'\mathbf{b}'\mathbf{c}']$ and $[\mathbf{abc}]$ of the two cells. $\det(\boldsymbol{S})$ is positive if the bases of the two cells have the same handedness and negative if they have opposite handedness.

If O and O' are the origins of the coordinate systems $(O, \mathbf{a}, \mathbf{b}, \mathbf{c})$ and $(O', \mathbf{a}', \mathbf{b}', \mathbf{c}')$, used for the description of $\mathcal{G}$ and $\mathcal{H}$, the column matrix of the coordinates of O' referred to the system $(O, \mathbf{a}, \mathbf{b}, \mathbf{c})$ will be denoted by $\boldsymbol{s}$. Thus, the coordinate system $(O', \mathbf{a}', \mathbf{b}', \mathbf{c}')$ will be specified completely by the square matrix $\boldsymbol{S}$ and the column matrix $\boldsymbol{s}$, symbolized by $\mathbb{S} : (\boldsymbol{S}, \boldsymbol{s})$.

An example of the application of equation (13.1.1.1) is given at the end of this chapter.

13.1.1.1. *The mathematical expression of equivalence*

Let $\mathbb{W} = (\boldsymbol{W}, \boldsymbol{w})$ be the operator of a given symmetry operation of $\mathcal{H}$ referred to $(O, \mathbf{a}, \mathbf{b}, \mathbf{c})$ and $\mathbb{W}' = (\boldsymbol{W}', \boldsymbol{w}')$ the operator of the same operation referred to $(O', \mathbf{a}', \mathbf{b}', \mathbf{c})$. Then the following relation applies

$$\mathbb{S}\mathbb{W}' = \mathbb{W}\mathbb{S} \quad \text{or} \quad \mathbb{W}' = \mathbb{S}^{-1}\mathbb{W}\mathbb{S} \qquad (13.1.1.2)$$

(*cf.* Bertaut & Billiet, 1979). The latter expression is more conventional, the former is easier to manipulate. Identifying the rotational (matrix) and translational (column) parts of $\mathbb{W}$, one obtains the following two conditions:

$$\begin{gathered} \boldsymbol{S}\boldsymbol{W}' = \boldsymbol{W}\boldsymbol{S}, \\ \boldsymbol{s} + \boldsymbol{S}\boldsymbol{w}' = \boldsymbol{w} + \boldsymbol{W}\boldsymbol{s} = \hat{\boldsymbol{w}} + \boldsymbol{t}_{\mathcal{G}} + \boldsymbol{W}\boldsymbol{s} \end{gathered} \qquad (13.1.1.2a)$$

or

$$\boldsymbol{S}\boldsymbol{w}' - \hat{\boldsymbol{w}} + (\boldsymbol{I} - \boldsymbol{W})\boldsymbol{s} = \boldsymbol{t}_{\mathcal{G}}. \qquad (13.1.1.2b)$$

Here we have split $\boldsymbol{w}$ into a fractional part $\hat{\boldsymbol{w}}$ (smaller than any lattice translation) and $\boldsymbol{t}_{\mathcal{G}}$ which describes a lattice translation in $\mathcal{G}$.

The general expression of the matrix $\boldsymbol{S}$ is

$$\boldsymbol{S} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix}. \qquad (13.1.1.3)$$

This general form, without any restrictions on the coefficients, applies only to the triclinic space groups $P1$ and $P\bar{1}$; $P1$ has only isomorphic subgroups (*cf.* Billiet, 1979; Billiet & Rolley Le Coz, 1980). For other space groups, restrictions have to be imposed on the coefficients S_{ij}.

13.1.2. Isomorphic subgroups

For convenience, we consider first those crystal systems that possess a unique direction (the privileged axis being taken parallel to **c**). We also include here the monoclinic system (unique axis either c or b).

13.1.2.1. *Monoclinic, tetragonal, trigonal, hexagonal systems*

If $\boldsymbol{W}$ is the matrix corresponding to a rotation about the c axis, $\boldsymbol{W}' = \boldsymbol{W}$ holds if the positive direction is the same for c and c'.† In consequence, $\boldsymbol{W}$ *must commute with* $\boldsymbol{S}$ [*cf.* equation (13.1.1.2*a*)]. This condition imposes relations on the coefficients S_{ij} of the matrix so that $\boldsymbol{S}$ and $\det(\boldsymbol{S})$ take the following forms:

Monoclinic system

$$\boldsymbol{M}_c = \begin{pmatrix} S_{11} & S_{12} & 0 \\ S_{21} & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{M}_c) = S_{33}(S_{11}S_{22} - S_{12}S_{21});$$

or if b instead of c is used

$$\boldsymbol{M}_b = \begin{pmatrix} S_{11} & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{M}_b) = S_{22}(S_{11}S_{33} - S_{13}S_{31}).$$

Tetragonal system

$$\boldsymbol{T}_1 = \begin{pmatrix} S_{11} & -S_{21} & 0 \\ S_{21} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{T}_1) = S_{33}(S_{11}^2 + S_{21}^2).$$

Hexagonal and trigonal systems

$$\boldsymbol{H}_1 = \begin{pmatrix} S_{11} & -S_{21} & 0 \\ S_{21} & S_{11} - S_{21} & 0 \\ 0 & 0 & S_{33} \end{pmatrix},$$

$$\det(\boldsymbol{H}_1) = S_{33}(S_{11}^2 + S_{21}^2 - S_{11}S_{21}).$$

For *rhombohedral* space groups, the matrix $\boldsymbol{H}_1$ applies only when hexagonal axes are used. If rhombohedral axes are used, the matrix $\boldsymbol{S}$ has the form

$$\boldsymbol{R}_1 = \begin{pmatrix} S_0 & S_2 & S_1 \\ S_1 & S_0 & S_2 \\ S_2 & S_1 & S_0 \end{pmatrix},$$

$$\begin{aligned} \det(\boldsymbol{R}_1) &= S_0^3 + S_1^3 + S_2^3 - 3S_0S_1S_2 \\ &= (S_0 + S_1 + S_2) \\ &\quad \times (S_0^2 + S_1^2 + S_2^2 - S_0S_1 - S_1S_2 - S_2S_0). \end{aligned}$$

* In general, this does not hold for non-isomorphic subgroups.

† If the positive directions of c and c' are opposite, $\boldsymbol{W}' = \boldsymbol{W}^{-1}$, but this does not bring in any new features.

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Table 13.1.2.1. *Isomorphic subgroups of the plane groups*

OBLIQUE SYSTEM

$$\boldsymbol{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{22} > 0, S_{11}S_{22} > 1, S_{21} = 0, -S_{11}/2 < S_{12} \leq S_{11}/2$

RECTANGULAR SYSTEM

$$\boldsymbol{O} = \begin{pmatrix} S_{11} & 0 \\ 0 & S_{22} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{22} > 0, S_{11}S_{22} > 1$

	$\boldsymbol{O}^a$	$\boldsymbol{O}^b$	$\boldsymbol{O}^c$	$\boldsymbol{O}^d$	$\boldsymbol{O}^e$
S_{11}	n_1	n_1	$2n_1 + 1$	$2n_1$	$2n_1 + 1$
S_{22}	n_2	$2n_2 + 1$	$2n_2 + 1$	$2n_2$	n_2

SQUARE SYSTEM

$$\boldsymbol{T}_1 = \begin{pmatrix} S_{11} & -S_{21} \\ S_{21} & S_{11} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{21} \geq 0, S_{11}^2 + S_{21}^2 > 1$

$$\boldsymbol{T}_2 = \begin{pmatrix} S_{11} & 0 \\ 0 & S_{11} \end{pmatrix}$$

Conditions: $\boldsymbol{T}_2^a : S_{11} > 1$; $\boldsymbol{T}_2^b : S_{11} = 2n_1 + 1 > 1$

$$\boldsymbol{T}_3 = \begin{pmatrix} S_{11} & -S_{11} \\ S_{11} & S_{11} \end{pmatrix}$$

Condition: $S_{11} > 0$

HEXAGONAL SYSTEM

$$\boldsymbol{H}_1 = \begin{pmatrix} S_{11} & -S_{21} \\ S_{21} & S_{11} - S_{21} \end{pmatrix}$$

Conditions: $S_{11} > 0, 0 \leq S_{21} < S_{11}, (S_{11}^2 + S_{21}^2 - S_{11}S_{21}) > 1$

$$\boldsymbol{H}_2 = \begin{pmatrix} S_{11} & 0 \\ 0 & S_{11} \end{pmatrix}$$

Condition: $S_{11} > 1$

$$\boldsymbol{H}_3 = \begin{pmatrix} 2S_{11} & -S_{11} \\ S_{11} & S_{11} \end{pmatrix}$$

Condition: $S_{11} > 0$

Table of plane subgroups

No. 1 $p1 : \boldsymbol{S}$; No. 2 $p2 : \boldsymbol{S}$; No. 3 $pm : \boldsymbol{O}^a$; No. 4 $pg : \boldsymbol{O}^b$;
No. 5 $cm : \boldsymbol{O}^c, \boldsymbol{O}^d$; No. 6 $p2mm : \boldsymbol{O}^a$; No. 7 $p2mg : \boldsymbol{O}^e$; No. 8 $p2gg : \boldsymbol{O}^c$;
No. 9 $c2mm : \boldsymbol{O}^c, \boldsymbol{O}^d$; No. 10 $p4 : \boldsymbol{T}_1$; No. 11 $p4mm : \boldsymbol{T}_2^a, \boldsymbol{T}_3$;
No. 12 $p4gm : \boldsymbol{T}_2^b$; No. 13 $p3 : \boldsymbol{H}_1$; No. 14 $p3m1 : \boldsymbol{H}_2$; No. 15 $p31m : \boldsymbol{H}_2$;
No. 16 $p6 : \boldsymbol{H}_1$; No. 17 $p6mm : \boldsymbol{H}_2, \boldsymbol{H}_3$.

13.1.2.1.1. *Additional restrictions*

If mirror or glide planes parallel to and/or twofold rotation or screw axes perpendicular to the principal rotation axis exist, further conditions are imposed upon the coefficients S_{ij} and these are indicated below (*cf.* Bertaut & Billiet, 1979).

Monoclinic system

The matrices $\boldsymbol{M}_c$ and $\boldsymbol{M}_b$ apply without any further restrictions on the coefficients.

Tetragonal system

The matrix $\boldsymbol{T}_1$ is valid for all space groups belonging to the crystal classes 4, $\bar{4}$ and $4/m$.

For all other space groups, restrictions apply to the coefficients S_{21} according to the following two rules which are consequences of equation (13.1.1.2*a*):

(i) If the last two letters of the Hermann–Mauguin symbol are different, $S_{21} = 0$; the corresponding matrix is called $\boldsymbol{T}_2$.

Example: $P4_2/mmc$

$$\boldsymbol{T}_2 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{T}_2) = S_{33}S_{11}^2.$$

(ii) If the last two letters are the same (except for the three cases mentioned below), two matrices have to be applied, the matrix $\boldsymbol{T}_2$ introduced above and the matrix $\boldsymbol{T}_1$ with $S_{21} = S_{11}$; the corresponding matrix is called $\boldsymbol{T}_3$.

$$\boldsymbol{T}_3 = \begin{pmatrix} S_{11} & -S_{11} & 0 \\ S_{11} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{T}_3) = 2S_{33}S_{11}^2.$$

The following space groups have matrices $\boldsymbol{T}_2$ and $\boldsymbol{T}_3$: $P422$, $P4mm$, $P4/mmm$, $P4_122$, $P4_322$, $P4_222$, $P4cc$, $P4/mcc$, $I422$, $I4mm$ and $I4/mmm$. The three exceptions to the rule mentioned above are the space groups $P4/nmm$, $P4/ncc$ and $I4_122$, which allow only $\boldsymbol{T}_2$.

Hexagonal and trigonal systems

The matrix $\boldsymbol{H}_1$ is valid for all space groups belonging to the crystal classes 6, $\bar{6}$, $6/m$, 3 and $\bar{3}$.

For all other space groups for which the last two letters of the Hermann–Mauguin symbol are different, $S_{22} = S_{11}$, and the matrix is called $\boldsymbol{H}_2$. Examples are $P6_3/mcm$, $P312$ and $P\bar{6}2m$.

$$\boldsymbol{H}_2 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{H}_2) = S_{33}S_{11}^2.$$

If the last two letters of the Hermann–Mauguin symbol are the same, two matrices have to be applied, the matrix $\boldsymbol{H}_2$ introduced above and the matrix $\boldsymbol{H}_1$ with $S_{11} = 2S'_{11}$ and $S_{21} = S'_{11}$; this matrix is called $\boldsymbol{H}_3$,

$$\boldsymbol{H}_3 = \begin{pmatrix} 2S'_{11} & -S'_{11} & 0 \\ S'_{11} & S'_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(\boldsymbol{H}_3) = 3S_{33}S'^2_{11}.$$

Examples are $P622$, $P6/mmm$ and $P6cc$.

Rhombohedral space groups

For $R3$ and $R\bar{3}$, one has the matrix $\boldsymbol{H}_1$ for hexagonal axes and $\boldsymbol{R}_1$ for rhombohedral axes. For all other rhombohedral space groups, one has $\boldsymbol{H}_2$ (hexagonal axes) and the matrix $\boldsymbol{R}_1$ with $S_1 = S_2$ (rhombohedral axes). This last matrix is called $\boldsymbol{R}_2$. Example: $R32$.

Table 13.1.2.2. *Isomorphic subgroups of the space groups*

TRICLINIC SYSTEM

$$\boldsymbol{S} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{22} > 0, S_{33} > 0, S_{11}S_{22}S_{33} > 1,$
$S_{21} = S_{31} = S_{32} = 0,\ -S_{11}/2 < S_{12} \le S_{11}/2,$
$-S_{11}/2 < S_{13} \le S_{11}/2,\ -S_{22}/2 < S_{23} \le S_{22}/2$

MONOCLINIC SYSTEM

Unique axis c

$$\boldsymbol{M}_c = \begin{pmatrix} S_{11} & S_{12} & 0 \\ S_{21} & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{33} > 0, (S_{11}S_{22} - S_{12}S_{21})S_{33} > 1$

	S_{11}	S_{12}	S_{21}	S_{22}	S_{33}	Extra condition
$\boldsymbol{M}_c^a$	$n_1 > 0$	0	n_3	$n_4 > 0$	n_5	$-n_4/2 < n_3 \le n_4/2$
$\boldsymbol{M}_c^b$	$n_1 > 0$	0	n_3	$n_4 > 0$	$2n_5 + 1$	$-n_4/2 < n_3 \le n_4/2$
$\boldsymbol{M}_c^c$	$n_1 > 0$	$2n_2$	0	$2n_4 + 1 > 0$	$2n_5 + 1$	$-n_1/2 < n_2 \le n_1/2$
$\boldsymbol{M}_c^d$	$n_1 > 0$	$2n_2$	0	$2n_4 > 0$	$2n_5$	$-n_1/2 < n_2 \le n_1/2$
$\boldsymbol{M}_c^e$	n_1	$2n_2 > 0$	$n_3 < 0$	0	$2n_5$	$-n_2 < n_1 \le n_2$
$\boldsymbol{M}_c^f$	$2n_1 + 1 > 0$	0	$2n_3$	$n_4 > 0$	n_5	$-n_4/2 < n_3 \le n_4/2$
$\boldsymbol{M}_c^g$	$2n_1 + 1 > 0$	$2n_2$	0	$2n_4 + 1 > 0$	$2n_5 + 1$	$-(2n_1 + 1)/2 < n_2 \le (2n_1 + 1)/2$
$\boldsymbol{M}_c^h$	$2n_1 + 1 > 0$	$2n_2$	0	$2n_4 > 0$	$2n_5$	$-(2n_1 + 1)/2 < n_2 \le (2n_1 + 1)/2$
$\boldsymbol{M}_c^i$	$2n_1 + 1$	$2n_2 > 0$	$n_3 < 0$	0	$2n_5$	$-(n_2 + 1)/2 < n_1 \le (n_2 - 1)/2$
$\boldsymbol{M}_c^j$	$2n_1 + 1 > 0$	0	$2n_3$	$n_4 > 0$	$2n_5 + 1$	$-n_4/2 < n_3 \le n_4/2$

Unique axis b

$$\boldsymbol{M}_b = \begin{pmatrix} S_{11} & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{22} > 0, (S_{11}S_{33} - S_{13}S_{31})S_{22} > 1$

	S_{11}	S_{13}	S_{22}	S_{31}	S_{33}	Extra condition
$\boldsymbol{M}_b^a$	$n_1 > 0$	n_2	n_3	0	$n_5 > 0$	$-n_1/2 < n_2 \le n_1/2$
$\boldsymbol{M}_b^b$	$n_1 > 0$	n_2	$2n_3 + 1$	0	$n_5 > 0$	$-n_1/2 < n_2 \le n_1/2$
$\boldsymbol{M}_b^c$	$2n_1 + 1 > 0$	0	$2n_3 + 1$	$2n_4$	$n_5 > 0$	$-n_5/2 < n_4 \le n_5/2$
$\boldsymbol{M}_b^d$	$2n_1 > 0$	0	$2n_3$	$2n_4$	$n_5 > 0$	$-n_5/2 < n_4 \le n_5/2$
$\boldsymbol{M}_b^e$	0	$n_2 < 0$	$2n_3$	$2n_4 > 0$	n_5	$-n_4 < n_5 \le n_4$
$\boldsymbol{M}_b^f$	n_1	$2n_2$	n_3	0	$2n_5 + 1 > 0$	$-n_1/2 < n_2 \le n_1/2$
$\boldsymbol{M}_b^g$	$2n_1 + 1 > 0$	0	$2n_3 + 1$	$2n_4$	$2n_5 + 1 > 0$	$-(2n_5 + 1)/2 < n_4 \le (2n_5 + 1)/2$
$\boldsymbol{M}_b^h$	$2n_1 > 0$	0	$2n_3$	$2n_4$	$2n_5 + 1 > 0$	$-(2n_5 + 1)/2 < n_4 \le (2n_5 + 1)/2$
$\boldsymbol{M}_b^i$	0	$n_2 < 0$	$2n_3$	$2n_4 > 0$	$2n_5 + 1$	$-(n_4 + 1)/2 < n_5 \le (n_4 - 1)/2$
$\boldsymbol{M}_b^j$	$n_1 > 0$	$2n_2$	$2n_3 + 1$	0	$2n_5 + 1 > 0$	$-n_1/2 < n_2 \le n_1/2$

$$\boldsymbol{R}_2 = \begin{pmatrix} S_0 & S_1 & S_1 \\ S_1 & S_0 & S_1 \\ S_1 & S_1 & S_0 \end{pmatrix}, \quad \det(\boldsymbol{R}_2) = (S_0 + 2S_1)(S_0 - S_1)^2.$$

13.1.2.2. *Cubic and orthorhombic systems*

Cubic system

For cubic space groups, equation (13.1.1.2*a*) leads to the matrix $\boldsymbol{C}$:

$$\boldsymbol{C} = \begin{pmatrix} S & 0 & 0 \\ 0 & S & 0 \\ 0 & 0 & S \end{pmatrix}, \quad \det(\boldsymbol{C}) = S^3.$$

Orthorhombic system

There are six choices of matrices $\boldsymbol{O}_i$ $(i = 1, 2, 3, 4, 5, 6)$ corresponding to the identical orientation ($\boldsymbol{O}_1$), to cyclic permutations of the three axes ($\boldsymbol{O}_2$ and $\boldsymbol{O}_3$) and to the interchange of two axes ($\boldsymbol{O}_4, \boldsymbol{O}_5$ and $\boldsymbol{O}_6$), *i.e.* to the six orthorhombic 'settings'.

$$\boldsymbol{O}_1 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}; \quad \boldsymbol{O}_2 = \begin{pmatrix} 0 & S_{12} & 0 \\ 0 & 0 & S_{23} \\ S_{31} & 0 & 0 \end{pmatrix};$$

$$\boldsymbol{O}_3 = \begin{pmatrix} 0 & 0 & S_{13} \\ S_{21} & 0 & 0 \\ 0 & S_{32} & 0 \end{pmatrix}; \quad \boldsymbol{O}_4 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & 0 & S_{23} \\ 0 & S_{32} & 0 \end{pmatrix};$$

$$\boldsymbol{O}_5 = \begin{pmatrix} 0 & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & 0 \end{pmatrix}; \quad \boldsymbol{O}_6 = \begin{pmatrix} 0 & S_{12} & 0 \\ S_{21} & 0 & 0 \\ 0 & 0 & S_{33} \end{pmatrix}.$$

The determinant is always equal to the product of the three non-zero coefficients, $\det(\boldsymbol{O}_i) = \pm S_{1j}S_{2k}S_{3l}$.

Table 13.1.2.2. *Isomorphic subgroups of the space groups* (*cont.*)

ORTHORHOMBIC SYSTEM

$$\boldsymbol{O}_1 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{22} > 0, S_{33} > 0, S_{11}S_{22}S_{33} > 1$

	S_{11}	S_{22}	S_{33}
$\boldsymbol{O}_1^a$	n_1	n_2	n_3
$\boldsymbol{O}_1^b$	n_1	n_2	$2n_3+1$
$\boldsymbol{O}_1^c$	$2n_1+1$	$2n_2+1$	n_3
$\boldsymbol{O}_1^d$	$2n_1+1$	$2n_2+1$	$2n_3+1$
$\boldsymbol{O}_1^e$	$2n_1$	$2n_2$	$2n_3+1$
$\boldsymbol{O}_1^f$	$2n_1$	$2n_2$	n_3
$\boldsymbol{O}_1^g$	$2n_1$	$2n_2$	$2n_3$
$\boldsymbol{O}_1^h$	$2n_1+1$	n_2	n_3
$\boldsymbol{O}_1^i$	$2n_1+1$	n_2	$2n_3+1$
$\boldsymbol{O}_1^j$	n_1	$2n_2+1$	$2n_3+1$
$\boldsymbol{O}_1^k$	n_1	$2n_2$	$2n_3$
$\boldsymbol{O}_1^l$	$2n_1+1$	$2n_2$	$2n_3$

$$\boldsymbol{O}_4 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & 0 & S_{23} \\ 0 & S_{32} & 0 \end{pmatrix}$$

Conditions: $S_{11} = 2n_1 > 0, S_{23} = -n_2 < 0, S_{32} = 2n_3 > 0$

$$\boldsymbol{O}_5 = \begin{pmatrix} 0 & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & 0 \end{pmatrix}$$

Conditions: $S_{13} = -n_1 < 0, S_{22} = 2n_2 > 0, S_{31} = 2n_3 > 0$

$$\boldsymbol{O}_6 = \begin{pmatrix} 0 & S_{12} & 0 \\ S_{21} & 0 & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{12} = 2n_1 > 0, S_{21} = -n_2 < 0, S_{33} = 2n_3 > 0$

The following general rule exists: only those matrices $\boldsymbol{O}_i$ are permissible for which, if the non-zero coefficients are replaced by 1, the corresponding transformation of the axes conserves the Hermann–Mauguin symbol.

Examples

(1) When the three letters of the Hermann–Mauguin symbol are the same, as in *P*222, *Pmmm*, *Pnnn etc.*, the Hermann–Mauguin symbol does not change and all six matrices are valid.

(2) When the *z* axis plays a privileged role and when the *x* and *y* axes are equivalent, only $\boldsymbol{O}_1$ and $\boldsymbol{O}_6$ apply. Examples are $P222_1$, *Pbam* and *Ccca*. In *Pmma*, the *x* and *y* axes are not equivalent because the interchange leads to *Pmmb* (the non-equivalence of the *x* and *y* axes can also be recognized by inspection of the full symbol $P2_1/m\ 2/m\ 2/a$).

(3) Matrix $\boldsymbol{O}_1$ always applies.

13.1.2.3. *Triclinic system*

As stated above, *P*1 has only isomorphic subgroups and the general nature of the matrix $\boldsymbol{S}$ [equation (13.1.1.3)] requires the use of special techniques (*cf.* Chapter 13.2, *Derivative lattices*); they apply also to $P\bar{1}$.

Table 13.1.2.2. *Isomorphic subgroups of the space groups* (*cont.*)

TETRAGONAL SYSTEM

$$\boldsymbol{T}_1 = \begin{pmatrix} S_{11} & -S_{21} & 0 \\ S_{21} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{21} \geq 0, S_{33} > 0, (S_{11}^2 + S_{21}^2)S_{33} > 1$

	S_{11}	S_{21}	S_{33}
$\boldsymbol{T}_1^a$	n_1	n_2	n_3
$\boldsymbol{T}_1^b$	n_1	n_2	$4n_3+1$
$\boldsymbol{T}_1^c$	n_1	n_2	$4n_3+3$
$\boldsymbol{T}_1^d$	n_1	n_2	$2n_3+1$
$\boldsymbol{T}_1^e$	$2n_1+1$	$2n_2$	$2n_3+1$
$\boldsymbol{T}_1^f$	$2n_1$	$2n_2+1$	$2n_3+1$
$\boldsymbol{T}_1^g$	$2n_1+1$	$2n_2+1$	$2n_3$
$\boldsymbol{T}_1^h$	$2n_1$	$2n_2$	$2n_3$
$\boldsymbol{T}_1^i$	$2n_1+1$	$2n_2$	n_3
$\boldsymbol{T}_1^j$	$2n_1$	$2n_2+1$	n_3

$$\boldsymbol{T}_2 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{33} > 0, S_{11}S_{33} > 1$

	S_{11}		S_{33}
$\boldsymbol{T}_2^a$	n_1		n_2
$\boldsymbol{T}_2^b$	$2n_1+1$		n_2
$\boldsymbol{T}_2^c$	n_1		$4n_2+1$
$\boldsymbol{T}_2^d$	n_1		$4n_2+3$
$\boldsymbol{T}_2^e$	$2n_1+1$		$4n_2+1$
$\boldsymbol{T}_2^f$	$2n_1+1$		$4n_2+3$
$\boldsymbol{T}_2^g$	n_1		$2n_2+1$
$\boldsymbol{T}_2^h$	$2n_1+1$		$2n_2+1$
$\boldsymbol{T}_2^i$	$2n_1$		$2n_2$

$$\boldsymbol{T}_3 = \begin{pmatrix} S_{11} & -S_{11} & 0 \\ S_{11} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions : $S_{11} > 0, S_{33} > 0$

$\boldsymbol{T}_3^a : S_{33} = n_1$; $\boldsymbol{T}_3^b : S_{33} = 4n_1 + 1$; $\boldsymbol{T}_3^c : S_{33} = 4n_1 + 1$;
$\boldsymbol{T}_3^d : S_{33} = 2n_1 + 1$; $\boldsymbol{T}_3^e : S_{33} = 2n_1$

13.1.2.4. *Parity conditions*

In equation (13.1.1.2*b*), there occurs the choice of the origin by means of *s*, the nature of the lattice by means of $\boldsymbol{t}_{\mathcal{G}}$ and the nature of the symmetry operations by means of the column matrices $\boldsymbol{w}$ and $\boldsymbol{w}'$. The three factors, origin, lattice type, screw and glide components, impose parity conditions on the coefficients of the matrix $\boldsymbol{S}$. Only a few examples are given here.

When $(\boldsymbol{W}, \boldsymbol{w})$ and $(\boldsymbol{W}', \boldsymbol{w}')$ are operators of lattice translations of $\mathcal{H}$, say $(\boldsymbol{I}, \boldsymbol{t}_{\mathcal{G}})$ and $(\boldsymbol{I}, \boldsymbol{t}_{\mathcal{H}})$, equation (13.1.1.2*b*) reduces to

$$\boldsymbol{S} \cdot \boldsymbol{t}_{\mathcal{H}} = \boldsymbol{t}_{\mathcal{G}}. \qquad (13.1.1.4)$$

Example

In a tetragonal *I* lattice, $\boldsymbol{t}_{\mathcal{G}}$ is either an integral or a fractional translation. If $\boldsymbol{t}_{\mathcal{H}}$ is $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and the matrix $\boldsymbol{S}$ is replaced by $\boldsymbol{T}_1$, one obtains

Table 13.1.2.2. *Isomorphic subgroups of the space groups* (*cont.*)

TRIGONAL AND HEXAGONAL SYSTEMS

Hexagonal axes

$$\boldsymbol{H}_1 = \begin{pmatrix} S_{11} & -S_{21} & 0 \\ S_{21} & S_{11}-S_{21} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, 0 \le S_{21} < S_{11}, S_{33} > 0, (S_{11}^2 + S_{21}^2 - S_{11}S_{21})S_{33} > 1$

$\boldsymbol{H}_1^a : S_{33} = n_1;\ \boldsymbol{H}_1^b : S_{33} = 3n_1 + 1;\ \boldsymbol{H}_1^c : S_{33} = 3n_1 + 2;$

$\boldsymbol{H}_1^d : S_{33} = 6n_1 + 1;\ \boldsymbol{H}_1^e : S_{33} = 6n_1 + 5;\ \boldsymbol{H}_1^f : S_{33} = 2n_3 + 1$

Conditions: $S_{11} > 0, S_{21} \ge 0, S_{33} > 0, (S_{11}^2 + S_{21}^2 - S_{11}S_{21})S_{33} > 1$

	S_{11}	S_{21}	S_{33}
$\boldsymbol{H}_1^g$	$3n_1 + 1$	$3n_2$	$3n_3 + 1$
$\boldsymbol{H}_1^h$	$3n_1 + 2$	$3n_2 + 2$	$3n_3 + 1$
$\boldsymbol{H}_1^i$	$3n_1$	$3n_2 + 1$	$3n_3 + 1$
$\boldsymbol{H}_1^j$	$3n_1 + 1$	$3n_2 + 1$	$3n_3 + 2$
$\boldsymbol{H}_1^k$	$3n_1 + 2$	$3n_2$	$3n_3 + 2$
$\boldsymbol{H}_1^l$	$3n_1$	$3n_2 + 2$	$3n_3 + 2$
$\boldsymbol{H}_1^m$	$3n_1 + 1$	$3n_2 + 2$	$3n_3$
$\boldsymbol{H}_1^n$	$3n_1 + 2$	$3n_2 + 1$	$3n_3$
$\boldsymbol{H}_1^o$	$3n_1$	$3n_2$	$3n_3$

$$\boldsymbol{H}_2 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{33} > 0, S_{11}S_{33} > 1$

	S_{11}		S_{33}
$\boldsymbol{H}_2^a$	n_1		n_2
$\boldsymbol{H}_2^b$	n_1		$3n_2 + 1$
$\boldsymbol{H}_2^c$	n_1		$3n_2 + 2$
$\boldsymbol{H}_2^d$	$3n_1 + 1$		$3n_2 + 1$
$\boldsymbol{H}_2^e$	$3n_1 + 2$		$3n_2 + 2$
$\boldsymbol{H}_2^f$	$3n_1$		$3n_2$
$\boldsymbol{H}_2^g$	n_1		$2n_2 + 1$
$\boldsymbol{H}_2^h$	$3n_1 + 1$		$6n_2 + 1$
$\boldsymbol{H}_2^i$	$3n_1 + 2$		$6n_2 + 5$
$\boldsymbol{H}_2^j$	$3n_1$		$6n_2 + 3$
$\boldsymbol{H}_2^k$	n_1		$6n_2 + 1$
$\boldsymbol{H}_2^l$	n_1		$6n_2 + 5$

$$\boldsymbol{H}_3 = \begin{pmatrix} 2S_{11} & -S_{11} & 0 \\ S_{11} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

Conditions: $S_{11} > 0, S_{33} > 0$

$\boldsymbol{H}_3^a : S_{33} = n_1;\ \boldsymbol{H}_3^b : S_{33} = 6n_1 + 1; \boldsymbol{H}_3^c : S_{33} = 6n_1 + 5;$

$\boldsymbol{H}_3^d : S_{33} = 3n_1 + 1; \boldsymbol{H}_3^e : S_{33} = 3n_1 + 2;\ \boldsymbol{H}_3^f : S_{33} = 2n_1 + 1$

Rhombohedral axes

$$\boldsymbol{R}_1 = \begin{pmatrix} S_0 & S_2 & S_1 \\ S_1 & S_0 & S_2 \\ S_2 & S_1 & S_0 \end{pmatrix}$$

Conditions: $S_0 > 0, S_1 \le S_0, -(S_0 + S_1) < S_2 < S_0,$

$(S_0 + S_1 + S_2)(S_0^2 + S_1^2 + S_2^2 - S_0S_1 - S_1S_2 - S_2S_0) > 1$

$$\boldsymbol{R}_2 = \begin{pmatrix} S_0 & S_1 & S_1 \\ S_1 & S_0 & S_1 \\ S_1 & S_1 & S_0 \end{pmatrix}$$

Conditions: $\boldsymbol{R}_2^a : S_0 > 0, -S_0/2 < S_1 < S_0;$

$\boldsymbol{R}_b^2 : S_0 > 0, -S_0/2 < S_1 < S_0, S_0 + 2S_1 = 2n + 1$

Table 13.1.2.2. *Isomorphic subgroups of the space groups* (*cont.*)

CUBIC SYSTEM

$$\boldsymbol{C} = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{11} \end{pmatrix}$$

Condition: $S_{11} > 1$

$\boldsymbol{C}^a : S_{11} = n_1;\ \boldsymbol{C}^b : S_{11} = 2n_1 + 1;$

$\boldsymbol{C}^c : S_{11} = 4n_1 + 1;\ \boldsymbol{C}^d : S_{11} = 4n_1 + 3$

Table of space subgroups

No. 1 $P1 : \boldsymbol{S}$; No. 2 $P\bar{1} : \boldsymbol{S}$; No. 3 $P112 : \boldsymbol{M}_c^a;\ P121 : \boldsymbol{M}_a^b;$
No. 4 $P112_1 : \boldsymbol{M}_c^b;\ P12_11 : \boldsymbol{M}_b^b$; No. 5 $A112 : \boldsymbol{M}_c^c, \boldsymbol{M}_c^d, \boldsymbol{M}_c^e;$
$C121 : \boldsymbol{M}_b^c, \boldsymbol{M}_b^d, \boldsymbol{M}_b^e$; No. 6 $P11m : \boldsymbol{M}_c^a;\ P1m1 : \boldsymbol{M}_b^a$; No. 7 $P11a : \boldsymbol{M}_c^f;$
$P1c1 : \boldsymbol{M}_b^f$; No. 8 $A11m : \boldsymbol{M}_c^c, \boldsymbol{M}_c^d, \boldsymbol{M}_c^e;\ C1m1 : \boldsymbol{M}_b^c, \boldsymbol{M}_b^d, \boldsymbol{M}_b^e;$
No. 9 $A11a : \boldsymbol{M}_c^g, \boldsymbol{M}_c^h, \boldsymbol{M}_c^i;\ C1c1 : \boldsymbol{M}_b^g, \boldsymbol{M}_b^h, \boldsymbol{M}_b^i$; No. 10 $P112/m : \boldsymbol{M}_c^a;$
$P12/m1 : \boldsymbol{M}_b^a$; No. 11 $P112_1/m : \boldsymbol{M}_c^b;\ P12_1/m1 : \boldsymbol{M}_b^b;$
No. 12 $A112/m : \boldsymbol{M}_c^c, \boldsymbol{M}_c^d, \boldsymbol{M}_c^e;\ C12/m1 : \boldsymbol{M}_b^c, \boldsymbol{M}_b^d, \boldsymbol{M}_b^e;$
No. 13 $P112/a : \boldsymbol{M}_c^f;\ P12/c1 : \boldsymbol{M}_b^f;$
No. 14 $P112_1/a : \boldsymbol{M}_c^j;\ P12_1/c1 : \boldsymbol{M}_b^j;$
No. 15 $A112/a : \boldsymbol{M}_c^g, \boldsymbol{M}_c^h, \boldsymbol{M}_c^i;\ C12/c1;\ \boldsymbol{M}_b^g, \boldsymbol{M}_b^h, \boldsymbol{M}_b^i$; No. 16 $P222 : \boldsymbol{O}_1^a;$
No. 17 $P222_1 : \boldsymbol{O}_1^b$; No. 18 $P2_12_12 : \boldsymbol{O}_1^c$; No. 19 $P2_12_12_1 : \boldsymbol{O}_1^d;$
No. 20 $C222_1 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^e$; No. 21 $C222 : \boldsymbol{O}_1^c, \boldsymbol{O}_1^f, \boldsymbol{O}_4, \boldsymbol{O}_5;$
No. 22 $F222 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^g$; No. 23 $I222 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^g$; No. 24 $I2_12_12_1 : \boldsymbol{O}_1^d;$
No. 25 $Pmm2 : \boldsymbol{O}_1^a$; No. 26 $Pmc2_1;\ \boldsymbol{O}_1^b$; No. 27 $Pcc2 : \boldsymbol{O}_1^b;$
No. 28 $Pma2 : \boldsymbol{O}_1^h$; No. 29 $Pca2_1 : \boldsymbol{O}_1^i$; No. 30 $Pnc2 : \boldsymbol{O}_1^j;$
No. 31 $Pmn2_1 : \boldsymbol{O}_1^i$; No. 32 $Pba2 : \boldsymbol{O}_1^c$; No. 33 $Pna2 : \boldsymbol{O}_1^d;$
No. 34 $Pnn2 : \boldsymbol{O}_1^d$; No. 35 $Cmm2 : \boldsymbol{O}_1^c, \boldsymbol{O}_1^f$; No. 36 $Cmc2_1 : \boldsymbol{O}_1^d;$
No. 37 $Ccc2 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^e$; No. 38 $Amm2 : \boldsymbol{O}_1^j, \boldsymbol{O}_1^k, \boldsymbol{O}_6$; No. 39 $Abm2 : \boldsymbol{O}_1^j;$
No. 40 $Ama2 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^l$; No. 41 $Aba2 : \boldsymbol{O}_1^d$; No. 42 $Fmm2 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^g;$
No. 43 $Fdd2 : \boldsymbol{O}_1^d$; No. 44 $Imm2 : \boldsymbol{O}_1^d, \boldsymbol{O}_1^g$; No. 45 $Iba2 : \boldsymbol{O}_1^d;$
No. 46 $Ima2 : \boldsymbol{O}_1^d$; No. 47 $Pmmm : \boldsymbol{O}_1^a$; No. 48 $Pnnn : \boldsymbol{O}_1^d;$
No. 49 $Pccm : \boldsymbol{O}_1^b$; No. 50 $Pban : \boldsymbol{O}_1^c$; No. 51 $Pmma : \boldsymbol{O}_1^h$
No. 52 $Pnna : \boldsymbol{O}_1^d$; No. 53 $Pmna : \boldsymbol{O}_1^i$; No. 54 $Pcca : \boldsymbol{O}_1^i;$
No. 55 $Pbam : \boldsymbol{O}_1^c$; No. 56 $Pccn : \boldsymbol{O}_1^d$; No. 57 $Pbcm : \boldsymbol{O}_1^j;$
No. 58 $Pnnm : \boldsymbol{O}_1^d$; No. 59 $Pmmn : \boldsymbol{O}_1^c$; No. 60 $Pbcn : \boldsymbol{O}_1^d;$
No. 61 $Pbca : \boldsymbol{O}_1^d$; No. 62 $Pnma : \boldsymbol{O}_1^d$; No. 63 $Cmcm : \boldsymbol{O}_1^d, \boldsymbol{O}_1^e;$
No. 64 $Cmca : \boldsymbol{O}_1^d$; No. 65 $Cmmm : \boldsymbol{O}_1^c, \boldsymbol{O}_1^f, \boldsymbol{O}_4, \boldsymbol{O}_5;$
No. 66 $Cccm : \boldsymbol{O}_1^d, \boldsymbol{O}_1^e$; No. 67 $Cmma : \boldsymbol{O}_1^c$; No. 68 $Ccca : \boldsymbol{O}_1^d;$
No. 69 $Fmmm : \boldsymbol{O}_1^d, \boldsymbol{O}_1^g$; No. 70 $Fddd : \boldsymbol{O}_1^d$; No. 71 $Immm : \boldsymbol{O}_1^d, \boldsymbol{O}_1^g;$
No. 72 $Ibam : \boldsymbol{O}_1^d$; No. 73 $Ibca : \boldsymbol{O}_1^d$; No. 74 $Imma : \boldsymbol{O}_1^d;$
No. 75 $P4 : \boldsymbol{T}_1^a$; No. 76 $P4_1 : \boldsymbol{T}_1^b$(subgroups $P4_1$), $\boldsymbol{T}_1^c$(subgroups $P4_3$);
No. 77 $P4_2 : \boldsymbol{T}_1^d$; No. 78 $P4_3 : \boldsymbol{T}_1^b$(subgroups $P4_3$), $\boldsymbol{T}_1^c$(subgroups $P4_1$);
No. 79 $I4 : \boldsymbol{T}_1^e, \boldsymbol{T}_1^f, \boldsymbol{T}_1^g, \boldsymbol{T}_1^h$; No. 80 $I4_1 : \boldsymbol{T}_1^e, \boldsymbol{T}_1^f$; No. 81 $P\bar{4} : \boldsymbol{T}_1^a;$
No. 82 $I\bar{4} : \boldsymbol{T}_1^e, \boldsymbol{T}_1^f, \boldsymbol{T}_1^g, \boldsymbol{T}_1^h$; No. 83 $P4/m : \boldsymbol{T}_1^a$; No. 84 $P4_2/m : \boldsymbol{T}_1^d;$
No. 85 $P4/n : \boldsymbol{T}_1^i, \boldsymbol{T}_1^j$; No. 86 $P4_2/n : \boldsymbol{T}_1^e, \boldsymbol{T}_1^f;$
No. 87 $I4/m : \boldsymbol{T}_1^e, \boldsymbol{T}_1^f, \boldsymbol{T}_1^g, \boldsymbol{T}_1^h$; No. 88 $I4_1/a : \boldsymbol{T}_1^e, \boldsymbol{T}_1^f;$
No. 89 $P422 : \boldsymbol{T}_2^a, \boldsymbol{T}_3^a$; No. 90 $P42_12 : \boldsymbol{T}_2^b;$
No. 91 $P4_122 : \boldsymbol{T}_2^c$(subgroups $P4_122$), $\boldsymbol{T}_2^d$(subgroups $P4_322$),
$\boldsymbol{T}_3^b$(subgroups $P4_122$), $\boldsymbol{T}_3^c$(subgroups $P4_322$);
No. 92 $P4_12_12 : \boldsymbol{T}_2^e$(subgroups $P4_12_12$), $\boldsymbol{T}_2^f$(subgroups $P4_32_12$);
No. 93 $P4_222 : \boldsymbol{T}_2^g, \boldsymbol{T}_3^d$; No. 94 $P4_22_12 : \boldsymbol{T}_2^h;$
No. 95 $P4_322 : \boldsymbol{T}_2^c$(subgroups $P4_322$), $\boldsymbol{T}_2^d$(subgroups $P4_122$),
$\boldsymbol{T}_3^b$(subgroups $P4_322$), $\boldsymbol{T}_3^c$(subgroups $P4_122$);
No. 96 $P4_32_12 : \boldsymbol{T}_2^e$(subgroups $P4_32_12$), $\boldsymbol{T}_2^f$(subgroups $P4_12_12$);
No. 97 $I422 : \boldsymbol{T}_2^h, \boldsymbol{T}_2^i, \boldsymbol{T}_3^e$; No. 98 $I4_122 : \boldsymbol{T}_2^h$; No. 99 $P4mm : \boldsymbol{T}_2^a, \boldsymbol{T}_3^a;$
No. 100 $P4bm : \boldsymbol{T}_2^b$; No. 101 $P4_2cm : \boldsymbol{T}_2^g$; No. 102 $P4_2nm : \boldsymbol{T}_2^h;$

Table 13.1.2.2. *Isomorphic subgroups of the space groups* (*cont.*)

Table of space subgroups (*cont.*)

No. 103 $P4cc$: $\boldsymbol{T}_2^g, \boldsymbol{T}_3^d$; No. 104 $P4nc$: $\boldsymbol{T}_2^h$; No. 105 $P4_2mc$: $\boldsymbol{T}_2^g$;
No. 106 $P4_2bc$: $\boldsymbol{T}_2^h$; No. 107 $I4mm$: $\boldsymbol{T}_2^h, \boldsymbol{T}_2^i, \boldsymbol{T}_3^e$; No. 108 $I4cm$: $\boldsymbol{T}_2^h$;
No. 109 $I4_1md$: $\boldsymbol{T}_2^h$; No. 110 $I4_1cd$: $\boldsymbol{T}_2^h$; No. 111 $P\bar{4}2m$: $\boldsymbol{T}_2^a$;
No. 112 $P\bar{4}2c$: $\boldsymbol{T}_2^g$; No. 113 $P\bar{4}2_1m$: $\boldsymbol{T}_2^h$; No. 114 $P\bar{4}2_1c$: $\boldsymbol{T}_2^h$;
No. 115 $P\bar{4}m2$: $\boldsymbol{T}_2^a$; No. 116 $P\bar{4}c2$: $\boldsymbol{T}_2^g$; No. 117 $P\bar{4}b2$: $\boldsymbol{T}_2^b$;
No. 118 $P\bar{4}n2$: $\boldsymbol{T}_2^h$; No. 119 $I\bar{4}m2$: $\boldsymbol{T}_2^h, \boldsymbol{T}_2^i$; No. 120 $I\bar{4}c2$: $\boldsymbol{T}_2^h$;
No. 121 $I\bar{4}2m$: $\boldsymbol{T}_2^h, \boldsymbol{T}_2^i$; No. 122 $I\bar{4}2d$: $\boldsymbol{T}_2^h$; No. 123 $P4/mmm$: $\boldsymbol{T}_2^a, \boldsymbol{T}_3^a$;
No. 124 $P4/mcc$: $\boldsymbol{T}_2^g, \boldsymbol{T}_3^d$; No. 125 $P4/nbm$: $\boldsymbol{T}_2^b$; No. 126 $P4/nnc$: $\boldsymbol{T}_2^h$;
No. 127 $P4/mbm$: $\boldsymbol{T}_2^b$; No. 128 $P4/mnc$: $\boldsymbol{T}_2^h$; No. 129 $P4/nmm$: $\boldsymbol{T}_2^b$;
No. 130 $P4/ncc$: $\boldsymbol{T}_2^h$; No. 131 $P4_2/mmc$: $\boldsymbol{T}_2^g$; No. 132 $P4_2/mcm$: $\boldsymbol{T}_2^g$;
No. 133 $P4_2/nbc$: $\boldsymbol{T}_2^h$; No. 134 $P4_2/nnm$: $\boldsymbol{T}_2^h$; No. 135 $P4_2/mbc$: $\boldsymbol{T}_2^h$;
No. 136 $P4_2/mnm$: $\boldsymbol{T}_2^h$; No. 137 $P4_2/nmc$: $\boldsymbol{T}_2^h$; No. 138 $P4_2/ncm$: $\boldsymbol{T}_2^h$;
No. 139 $I4/mmm$: $\boldsymbol{T}_2^h, \boldsymbol{T}_2^i, \boldsymbol{T}_3^e$; No. 140 $I4/mcm$: $\boldsymbol{T}_2^h$;
No. 141 $I4_1/amd$: $\boldsymbol{T}_2^h$; No. 142 $I4_1/acd$: $\boldsymbol{T}_2^h$; No. 143 $P3$: $\boldsymbol{H}_1^a$;
No. 144 $P3_1$: $\boldsymbol{H}_1^b$(subgroups $P3_1$), $\boldsymbol{H}_1^c$(subgroups $P3_2$);
No. 145 $P3_2$: $\boldsymbol{H}_1^b$(subgroups $P3_2$), $\boldsymbol{H}_1^c$(subgroups $P3_1$);
No. 146 $R3$ (hexagonal axes): $\boldsymbol{H}_1^g, \boldsymbol{H}_1^h, \boldsymbol{H}_1^i, \boldsymbol{H}_1^j, \boldsymbol{H}_1^k, \boldsymbol{H}_1^l, \boldsymbol{H}_1^m, \boldsymbol{H}_1^n, \boldsymbol{H}_1^o$;
$R3$ (rhombohedral axes): $\boldsymbol{R}_1$; No. 147 $P\bar{3}$: $\boldsymbol{H}_1^a$;
No. 148 $R\bar{3}$ (hexagonal axes): $\boldsymbol{H}_1^g, \boldsymbol{H}_1^h, \boldsymbol{H}_1^i, \boldsymbol{H}_1^j, \boldsymbol{H}_1^k, \boldsymbol{H}_1^l, \boldsymbol{H}_1^m, \boldsymbol{H}_1^n, \boldsymbol{H}_1^o$;
$R\bar{3}$ (rhombohedral axes): $\boldsymbol{R}_1$; No. 149 $P312$: $\boldsymbol{H}_2^a$; No. 150 $P321$: $\boldsymbol{H}_2^a$;
No. 151 $P3_112$: $\boldsymbol{H}_2^b$(subgroups $P3_112$), $\boldsymbol{H}_2^c$(subgroups $P3_212$);
No. 152 $P3_121$: $\boldsymbol{H}_2^b$(subgroups $P3_121$), $\boldsymbol{H}_2^c$(subgroups $P3_221$);
No. 153 $P3_212$: $\boldsymbol{H}_2^b$(subgroups $P3_212$), $\boldsymbol{H}_2^c$(subgroups $P3_112$);
No. 154 $P3_221$: $\boldsymbol{H}_2^b$(subgroups $P3_221$), $\boldsymbol{H}_2^c$(subgroups $P3_121$);
No. 155 $R32$ (hexagonal axes): $\boldsymbol{H}_2^d, \boldsymbol{H}_2^e, \boldsymbol{H}_2^f$; $R32$ (rhombohedral axes):
$\boldsymbol{R}_2^a$; No. 156 $P3m1$: $\boldsymbol{H}_2^a$; No. 157 $P31m$: $\boldsymbol{H}_2^a$; No. 158 $P3c1$: $\boldsymbol{H}_2^g$;
No. 159 $P31c$: $\boldsymbol{H}_2^g$; No. 160 $R3m$ (hexagonal axes): $\boldsymbol{H}_2^d, \boldsymbol{H}_2^e, \boldsymbol{H}_2^f$;
$R3m$ (rhombohedral axes): $\boldsymbol{R}_2^a$; No. 161 $R3c$ (hexagonal axes):
$\boldsymbol{H}_2^h, \boldsymbol{H}_2^i, \boldsymbol{H}_2^j$; $R3c$ (rhombohedral axes): $\boldsymbol{R}_2^b$; No. 162 $P\bar{3}1m$: $\boldsymbol{H}_2^a$;
No. 163 $P\bar{3}1c$: $\boldsymbol{H}_2^g$; No. 164 $P\bar{3}m1$: $\boldsymbol{H}_2^a$; No. 165 $P\bar{3}c1$: $\boldsymbol{H}_2^g$;
No. 166 $R\bar{3}m$ (hexagonal axes): $\boldsymbol{H}_2^d, \boldsymbol{H}_2^e, \boldsymbol{H}_2^f$; $R\bar{3}m$ (rhombohedral
axes): $\boldsymbol{R}_2^a$; No. 167 $R\bar{3}c$ (hexagonal axes): $\boldsymbol{H}_2^h, \boldsymbol{H}_2^i, \boldsymbol{H}_2^j$;
$R\bar{3}c$ (rhombohedral axes): $\boldsymbol{R}_2^b$; No. 168 $P6$: $\boldsymbol{H}_1^a$;
No. 169 $P6_1$: $\boldsymbol{H}_1^d$(subgroups $P6_1$), $\boldsymbol{H}_1^e$(subgroups $P6_5$);
No. 170 $P6_5$: $\boldsymbol{H}_1^d$(subgroups $P6_5$), $\boldsymbol{H}_1^e$(subgroups $P6_1$);
No. 171 $P6_2$: $\boldsymbol{H}_1^b$(subgroups $P6_2$), $\boldsymbol{H}_1^c$(subgroups $P6_4$);
No. 172 $P6_4$: $\boldsymbol{H}_1^b$(subgroups $P6_4$), $\boldsymbol{H}_1^c$(subgroups $P6_2$);
No. 173 $P6_3$: $\boldsymbol{H}_1^f$; No. 174 $P\bar{6}$: $\boldsymbol{H}_1^a$; No. 175 $P6/m$: $\boldsymbol{H}_1^a$;
No. 176 $P6_3/m$: $\boldsymbol{H}_1^f$; No. 177 $P622$: $\boldsymbol{H}_2^a$; $\boldsymbol{H}_3^a$;
No. 178 $P6_122$: $\boldsymbol{H}_2^k$(subgroups $P6_122$), $\boldsymbol{H}_2^l$(subgroups $P6_522$),
$\boldsymbol{H}_3^b$(subgroups $P6_122$), $\boldsymbol{H}_3^c$(subgroups $P6_522$);
No. 179 $P6_522$: $\boldsymbol{H}_2^k$(subgroups $P6_522$), $\boldsymbol{H}_2^l$(subgroups $P6_122$),
$\boldsymbol{H}_3^b$(subgroups $P6_522$), $\boldsymbol{H}_3^c$(subgroups $P6_122$);
No. 180 $P6_222$: $\boldsymbol{H}_2^b$(subgroups $P6_222$), $\boldsymbol{H}_2^c$(subgroups $P6_422$),
$\boldsymbol{H}_3^d$(subgroups $P6_222$), $\boldsymbol{H}_3^e$(subgroups $P6_422$);
No. 181 $P6_422$: $\boldsymbol{H}_2^b$(subgroups $P6_422$), $\boldsymbol{H}_2^c$(subgroups $P6_222$),
$\boldsymbol{H}_3^d$(subgroups $P6_422$), $\boldsymbol{H}_3^e$(subgroups $P6_222$); No. 182 $P6_322$: $\boldsymbol{H}_2^g, \boldsymbol{H}_3^f$;
No. 183 $P6mm$: $\boldsymbol{H}_2^a, \boldsymbol{H}_3^a$; No. 184 $P6cc$: $\boldsymbol{H}_2^g, \boldsymbol{H}_3^f$; No. 185 $P6_3cm$: $\boldsymbol{H}_2^g$;
No. 186 $P6_3mc$: $\boldsymbol{H}_2^g$; No. 187 $P\bar{6}m2$: $\boldsymbol{H}_2^a$; No. 188 $P\bar{6}c2$: $\boldsymbol{H}_2^g$;
No. 189 $P\bar{6}2m$: $\boldsymbol{H}_2^a$; No. 190 $P\bar{6}2c$: $\boldsymbol{H}_2^g$; No. 191 $P6/mmm$: $\boldsymbol{H}_2^a, \boldsymbol{H}_3^a$;
No. 192 $P6/mcc$: $\boldsymbol{H}_2^g, \boldsymbol{H}_3^f$; No. 193 $P6_3/mcm$: $\boldsymbol{H}_2^g$;
No. 194 $P6_3/mmc$: $\boldsymbol{H}_2^g$; No. 195 $P23$: $\boldsymbol{C}^a$; No. 196 $F23$: $\boldsymbol{C}^a$;
No. 197 $I23$: $\boldsymbol{C}^a$; No. 198 $P2_13$: $\boldsymbol{C}^b$; No. 199 $I2_13$: $\boldsymbol{C}^b$;
No. 200 $Pm\bar{3}$: $\boldsymbol{C}^a$; No. 201 $Pn\bar{3}$: $\boldsymbol{C}^b$; No. 202 $Fm\bar{3}$: $\boldsymbol{C}^a$;
No. 203 $Fd\bar{3}$: $\boldsymbol{C}^b$; No. 204 $Im\bar{3}$: $\boldsymbol{C}^a$; No. 205 $Pa\bar{3}$: $\boldsymbol{C}^b$;
No. 206 $Ia\bar{3}$: $\boldsymbol{C}^b$; No. 207 $P432$: $\boldsymbol{C}^a$; No. 208 $P4_232$: $\boldsymbol{C}^b$;

Table 13.1.2.2. *Isomorphic subgroups of the space groups* (*cont.*)

Table of space subgroups (*cont.*)

No. 209 $F432$: $\boldsymbol{C}^a$; No. 210 $F4_132$: $\boldsymbol{C}^b$; No. 211 $I432$: $\boldsymbol{C}^a$;
No. 212 $P4_332$: $\boldsymbol{C}^c$(subgroups $P4_332$), $\boldsymbol{C}^d$(subgroups $P4_132$);
No. 213 $P4_132$: $\boldsymbol{C}^c$(subgroups $P4_132$), $\boldsymbol{C}^d$(subgroups $P4_332$);
No. 214 $I4_132$: $\boldsymbol{C}^b$; No. 215 $P\bar{4}3m$: $\boldsymbol{C}^a$; No. 216 $F\bar{4}3m$: $\boldsymbol{C}^a$;
No. 217 $I\bar{4}3m$: $\boldsymbol{C}^a$: No. 218 $P\bar{4}3n$: $\boldsymbol{C}^b$; No. 219 $F\bar{4}3c$: $\boldsymbol{C}^b$;
No. 220 $I\bar{4}3d$: $\boldsymbol{C}^b$; No. 221 $Pm\bar{3}m$: $\boldsymbol{C}^a$; No. 222 $Pn\bar{3}n$: $\boldsymbol{C}^b$;
No. 223 $Pm\bar{3}n$: $\boldsymbol{C}^b$; No. 224 $Pn\bar{3}m$: $\boldsymbol{C}^b$; No. 225 $Fm\bar{3}m$: $\boldsymbol{C}^a$;
No. 226 $Fm\bar{3}c$: $\boldsymbol{C}^b$; No. 227 $Fd\bar{3}m$: $\boldsymbol{C}^b$; No. 228 $Fd\bar{3}c$: $\boldsymbol{C}^b$;
No. 229 $Im\bar{3}m$: $\boldsymbol{C}^a$; No. 230 $Ia\bar{3}d$: $\boldsymbol{C}^b$.

$$\boldsymbol{S}\begin{pmatrix}\frac{1}{2}\\ \frac{1}{2}\\ \frac{1}{2}\end{pmatrix} = \begin{pmatrix}\frac{1}{2}(S_{11}-S_{21})\\ \frac{1}{2}(S_{11}+S_{21})\\ \frac{1}{2}S_{33}\end{pmatrix} = \begin{pmatrix}n_1\\ n_2\\ n_3\end{pmatrix} \text{ or } \begin{pmatrix}n_1+\frac{1}{2}\\ n_2+\frac{1}{2}\\ n_3+\frac{1}{2}\end{pmatrix} \qquad (13.1.1.4a)$$

with n_1, n_2, n_3 integers.

From this it follows that either S_{11} and S_{21} have the same parity and S_{33} is even, or else S_{11} and S_{21} have opposite parities and S_{33} is odd.

If $(\boldsymbol{W}, \boldsymbol{w})$ and $(\boldsymbol{W}', \boldsymbol{w}')$ represent the same operation 4_1 in the two P lattices of $\mathcal{G}$ and $\mathcal{H}$, with $\hat{\boldsymbol{w}} = \boldsymbol{w}' = (00\frac{1}{4})$, for $\boldsymbol{s} = \boldsymbol{0}$, equation (13.1.1.2*b*) reduces to

$$\tfrac{1}{4}(S_{33}-1) = n \quad \text{or} \quad S_{33} = 4n+1, \quad n \text{ integer}.$$

There are similar conditions for glide and other screw operations.

The location part $\boldsymbol{s}$, *i.e.* the relative positions of the origins O and O' of group and subgroup, is another important problem. This problem can be approached in two ways. First, only standard settings and origins (as defined in the space-group tables of this volume) of the group $\mathcal{G}$ and its subgroup $\mathcal{H}$ are considered. In this case, the origin relation between $\mathcal{G}$ and $\mathcal{H}$ must be indicated by the appropriate column $\boldsymbol{s}$. For instance, in $P2_12_12_1$ the matrices $\boldsymbol{O}_4, \boldsymbol{O}_5, \boldsymbol{O}_6$ are only possible for $s \neq o$, say $s = (-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4})$. Second, one can describe $\mathcal{H}$ based on the same origin as $\mathcal{G}$, *i.e.* O and O' coincide. In this case, nonstandard descriptions of $\mathcal{H}$ frequently result and one has to indicate the location of the symmetry elements of $\mathcal{H}$ with respect to the origin of $\mathcal{G}$.

Unfortunately, it was not possible to incorporate in the present tables the implications that the choice of the origin has on the coefficients S_{ij} (*cf.* Bertaut, 1956; Billiet, 1978; Bertaut & Billiet, 1979).

The explicit forms of the matrices $\boldsymbol{S}$ for each space group and each plane group are given in Tables 13.1.2.1 and 13.1.2.2 without origin indications.

Example

Consider space groups $P4/mmm$ and $P4/mcc$ and envisage the matrix $\boldsymbol{T}_3$ which has the determinant $2S_{33}S_{11}^2$. Its lowest value is 2 with $S_{11} = S_{33} = 1$. The matrix $\boldsymbol{T}_3$ then implies the axis transformation

$$\mathbf{a}' = \mathbf{a} + \mathbf{b}, \quad \mathbf{b}' = -\mathbf{a} + \mathbf{b}, \quad \mathbf{c}' = \mathbf{c}.$$

Envisage also the matrix $\boldsymbol{T}_2$ which has the determinant $S_{11}^2 S_{33}$. Its lowest value for a proper subgroup is 2 with $S_{11} = 1$ and $S_{33} = 2$. The axis transformation is here

$$\mathbf{a}' = \mathbf{a}, \quad \mathbf{b}' = \mathbf{b}, \quad \mathbf{c}' = 2\mathbf{c}.$$

This transformation is permitted for $P4/mmm$ but not for $P4/mcc$ where the parity rules require $S_{33} = 2n + 1$. Thus, the lowest value of $S_{11}^2 S_{33}$ for a subgroup of space group $P4/mcc$ is 3 and the axis transformation is

$$\mathbf{a}' = \mathbf{a}, \quad \mathbf{b}' = \mathbf{b}, \quad \mathbf{c}' = 3\mathbf{c}.$$

13.1.2.5. *Plane groups*

There is no difficulty in reducing the preceding considerations to plane groups, where $\boldsymbol{S}$ is a (2×2) matrix and $\boldsymbol{s}$ a (2×1) matrix.

13.1.2.6. *Tables of matrices for isomorphic subgroups*

The matrices and the restrictions on the coefficients are listed for the plane groups in Table 13.1.2.1 and for the space groups in Table 13.1.2.2.

For the triclinic and monoclinic systems, there is an infinite choice of matrices for each index, owing to the infinite number of equivalent unit cells. For the other space groups, several different (but finitely many) choices of matrix occur. In all cases, we have restricted this choice to *one* matrix for each group–subgroup relation so that *each subgroup is listed exactly once* (apart from origin choice).

Example

No. 178, $P6_122$, has the matrix $\boldsymbol{H}_2^k$ for *all isomorphic and isosymbolic* subgroups $P6_122$, having the lattices $n_{11}\mathbf{a}$, $n_{11}\mathbf{b}$, $(6n_{33} + 1)\mathbf{c}$ $(n_{11} \geq 1, n_{33} \geq 0)$, whilst $\boldsymbol{H}_3^b$ is used for *all isomorphic and isosymbolic* subgroups with the lattices $n_{11}(2\mathbf{a} + \mathbf{b})$, $n_{11}(-\mathbf{a} + \mathbf{b})$, $(6n_{33} + 1)\mathbf{c}$ $(n_{11} \geq 1, n_{33} \geq 0)$. These two kinds of subgroups are obviously different, having different translation lattices. The same group, $P6_122$, has the matrix $\boldsymbol{H}_2^l$ for the *isomorphic and enantiomorphic subgroups* $P6_522$ of lattices $n_{11}\mathbf{a}$, $n_{11}\mathbf{b}$, $(6n_{33} + 5)\mathbf{c}$ whilst $\boldsymbol{H}_3^c$ is used for the *isomorphic and enantiomorphic subgroups* $P6_522$ of lattices $n_{11}(2\mathbf{a} + \mathbf{b})$, $n_{11}(-\mathbf{a} + \mathbf{b})$, $(6n_{33} + 5)\mathbf{c}$.

In the tables, each system is preceded by the appropriate general form of the matrix, which is also given in this chapter, followed by the more specialized matrices such as $\boldsymbol{T}_2, \boldsymbol{T}_3$. Under *Conditions*, we have listed the nonredundant inequalities and parity conditions* that ensure the uniqueness of the matrix for each subgroup. Also, we have used rules in order to avoid repetition of equivalent unit cells. For instance, for trigonal and hexagonal groups (rhombohedral groups excepted), we have restricted $\mathbf{a}'$ to lie between $\mathbf{a}$ and $\mathbf{a} + \mathbf{b}$ excluding this last vector from the sector of 60° because there is a repetition after a 60° rotation of the unit cell.

* More exactly 'congruence modulo $\mathbb{Z}$ conditions'.

Table 13.2.2.1. *Three-dimensional derivative lattices of indices 2 to 7* (*cont.*)

Index 7	1(7**a**, **b**, **c**); 2(**a**, 7**b**, **c**); 3(**a**, **b**, 7**c**); 4(7**a**, **b** + **a**, **c**); 5(7**a**, **b**, **c** + **b**); 6(**a**, 7**b**, **c** + **b**); 7(7**a**, **b** − **a**, **c**); 8(7**a**, **b**, **c** − **a**); 9(**a**, 7**b**, **c** − **b**); 10(7**a**, **b** + 2**a**, **c**); 11(7**a**, **b**, **c** − 3**a**); 12(**a**, 7**b**, **c** + 2**b**); 13(7**a**, **b** − 3**a**, **c**); 14(7**a**, **b**, **c** + 2**a**); 15(**a**, 7**b**, **c** − 3**b**); 16(7**a**, **b** − 2**a**, **c**); 17(7**a**, **b**, **c** + 3**a**); 18(**a**, 7**b**, **c** − 2**b**); 19(7**a**, **b** + 3**a**, **c**); 20(7**a**, **b**, **c** − 2**a**); 21(**a**, 7**b**, **c** + 3**b**); 22(7**a**, **b** + **a**, **c** + **a**); 23(7**a**, **b** + **a**, **c** − **a**); 24(7**a**, **b** − **a**, **c** + **a**); 25(7**a**, **b** − **a**, **c** − **a**); 26(7**a**, **b** + **a**, **c** + 2**a**); 27(7**a**, **b** + **a**, **c** − 2**a**); 28(7**a**, **b** + 2**a**, **c** + **a**); 29(7**a**, **b** − 2**a**, **c** + **a**); 30(7**a**, **b** + 3**a**, **c** − 3**a**); 31(7**a**, **b** − 3**a**, **c** + 3**a**); 32(7**a**, **b** + **a**, **c** + 3**a**); 33(7**a**, **b** + **a**, **c** − 3**a**); 34(7**a**, **b** + 3**a**, **c** + **a**); 35(7**a**, **b** − 3**a**, **c** + **a**); 36(7**a**, **b** + 2**a**, **c** − 2**a**); 37(7**a**, **b** − 2**a**, **c** + 2**a**); 38(7**a**, **b** + 2**a**, **c** + 2**a**); 39(7**a**, **b** − 3**a**, **c** − **a**); 40(7**a**, **b** − **a**, **c** − 3**a**); 41(7**a**, **b** − 2**a**, **c** − 2**a**); 42(7**a**, **b** + 3**a**, **c** − **a**); 43(7**a**, **b** − **a**, **c** + 3**a**); 44(7**a**, **b** + 2**a**, **c** + 3**a**); 45(7**a**, **b** + 3**a**, **c** + 2**a**); 46(7**a**, **b** − 2**a**, **c** − 3**a**); 47(7**a**, **b** − 3**a**, **c** + 2**a**); 48(7**a**, **b** + 2**a**, **c** − 3**a**); 49(7**a**, **b** − 3**a**, **c** − 2**a**); 50(7**a**, **b** − 2**a**, **c** + 3**a**); 51(7**a**, **b** + 3**a**, **c** − 2**a**); 52(7**a**, **b** + 3**a**, **c** + 3**a**); 53(7**a**, **b** − 2**a**, **c** − **a**); 54(7**a**, **b** − **a**, **c** − 2**a**); 55(7**a**, **b** − 3**a**, **c** − 3**a**); 56(7**a**, **b** + 2**a**, **c** − **a**); 57(7**a**, **b** − **a**, **c** + 2**a**)

Example

One can derive easily the 7 derivative lattices of index 2.

$$1(2\mathbf{a},\mathbf{b},\mathbf{c});\ 2(\mathbf{a},2\mathbf{b},\mathbf{c});\ 3(\mathbf{a},\mathbf{b},2\mathbf{c});\ 4(2\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c});$$
$$5(2\mathbf{a},\mathbf{b},\mathbf{c}+\mathbf{a});\ 6(\mathbf{a},2\mathbf{b},\mathbf{c}+\mathbf{b});\ 7(2\mathbf{a},\mathbf{b}+\mathbf{a},\mathbf{c}+\mathbf{a}).$$

Another primitive cell of a given derivative lattice is obtained if one of the following three elementary transformations is performed on the vectors of a primitive cell of this derivative lattice:

(i) the sign of a vector is changed;
(ii) two vectors are interchanged;
(iii) to a vector is added q times another vector (q integer).

(i) and (ii) are left-handed transformations, (iii) is right-handed.

Example

The primitive cell $\mathbf{a}'', \mathbf{b}'', \mathbf{c}''$ ($\mathbf{a}'' = -2\mathbf{b} - \mathbf{a}, \mathbf{b}'' = 9\mathbf{a} - 2\mathbf{c} - 2\mathbf{b}, \mathbf{c}'' = \mathbf{c} - \mathbf{a} + 3\mathbf{b}$) belongs to the derivative lattice of index 10 given by the primitive cell $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ ($\mathbf{a}' = 5\mathbf{a},\ \mathbf{b}' = 2\mathbf{b} + \mathbf{a},\ \mathbf{c}' = \mathbf{c} - 2\mathbf{a} + \mathbf{b}$) because these two cells are related by the following sequence of elementary transformations:

$$(-2\mathbf{b}-\mathbf{a},\ 9\mathbf{a}-2\mathbf{c}-2\mathbf{b},\ \mathbf{c}-\mathbf{a}+3\mathbf{b}) \overset{\text{(iii)}}{\rightarrow}$$
$$(-2\mathbf{b}-\mathbf{a},\ 9\mathbf{a}-2\mathbf{c}-2\mathbf{b},\ \mathbf{c}-2\mathbf{a}+\mathbf{b}) \overset{\text{(iii)}}{\rightarrow}$$
$$(-2\mathbf{b}-\mathbf{a},\ 5\mathbf{a},\ \mathbf{c}-2\mathbf{a}+\mathbf{b}) \overset{\text{(i)}}{\rightarrow} (2\mathbf{b}+\mathbf{a},\ 5\mathbf{a},\ \mathbf{c}-2\mathbf{a}+\mathbf{b})$$
$$\overset{\text{(ii)}}{\rightarrow} (5\mathbf{a},\ 2\mathbf{b}+\mathbf{a},\ \mathbf{c}-2\mathbf{a}+\mathbf{b});$$

($\mathbf{a}''$, $\mathbf{b}''$, $\mathbf{c}''$) and ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$) have the same handedness.

13.2.3. Two-dimensional derivative lattices

All previous considerations are valid also for two-dimensional lattices and their derivative lattices (Table 13.2.3.1). The relevant formula for any index is

$$\mathbf{a}' = p_1\mathbf{a}, \quad \mathbf{b}' = p_2\mathbf{b} + q\mathbf{a}$$
$$[\mathbf{a} \text{ direction is kept}]$$
$$(p_1, p_2 \text{ positive integers, not necessarily prime;}$$
$$\text{index} = p_1p_2 > 1;\ q \text{ any integer}; -p_1/2 < q \le p_1/2).$$

A similar formula is obtained by interchange of **a** and **b**.

Table 13.2.3.1. *Two-dimensional derivative lattices of indices 2 to 7*

The entry for each derivative lattice starts with a running number which is followed, between parentheses, by the appropriate basis-vector relations.

Index 2	1(2**a**, **b**); 2(**a**, 2**b**); 3(2**a**, **b** + **a**)
Index 3	1(3**a**, **b**); 2(**a**, 3**b**); 3(3**a**, **b** + **a**); 4(3**a**, **b** − **a**)
Index 4	1(4**a**, **b**); 2(**a**, 4**b**); 3(4**a**, **b** + **a**); 4(4**a**, **b** − **a**); 5(4**a**, **b** + 2**a**); 6(2**a**, 2**b** + **a**); 7(2**a**, 2**b**)
Index 5	1(5**a**, **b**); 2(**a**, 5**b**); 3(5**a**, **b** + **a**); 4(5**a**, **b** − **a**); 5(5**a**, **b** + 2**a**); 6(5**a**, **b** − 2**a**)
Index 6	1(6**a**, **b**); 2(**a**, 6**b**); 3(6**a**, **b** + **a**); 4(6**a**, **b** − **a**); 5(6**a**, **b** + 2**a**); 6(3**a**, 2**b** + **a**); 7(6**a**, **b** − 2**a**); 8(3**a**, 2**b** − **a**); 9(6**a**, **b** + 3**a**); 10(2**a**, 3**b** + **a**); 11(3**a**, 2**b**); 12(2**a**, 3**b**)
Index 7	1(7**a**, **b**); 2(**a**, 7**b**); 3(7**a**, **b** + **a**); 4(7**a**, **b** − **a**); 5(7**a**, **b** + 2**a**); 6(7**a**, **b** − 3**a**); 7(7**a**, **b** − 2**a**); 8(7**a**, **b** + 3**a**)

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