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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

$$O_1 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

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

	S_{11}	S_{22}	S_{33}
O_1^a	n_1	n_2	n_3
O_1^b	n_1	n_2	$2n_3 + 1$
O_1^c	$2n_1 + 1$	$2n_2 + 1$	n_3
O_1^d	$2n_1 + 1$	$2n_2 + 1$	$2n_3 + 1$
O_1^e	$2n_1$	$2n_2$	$2n_3 + 1$
O_1^f	$2n_1$	$2n_2$	n_3
O_1^g	$2n_1$	$2n_2$	$2n_3$
O_1^h	$2n_1 + 1$	n_2	n_3
O_1^i	$2n_1 + 1$	n_2	$2n_3 + 1$
O_1^j	n_1	$2n_2 + 1$	$2n_3 + 1$
O_1^k	n_1	$2n_2$	$2n_3$
O_1^l	$2n_1 + 1$	$2n_2$	$2n_3$

$$O_4 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & 0 & S_{23} \\ 0 & S_{32} & 0 \end{pmatrix}$$

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

$$O_5 = \begin{pmatrix} 0 & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & 0 \end{pmatrix}$$

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

$$O_6 = \begin{pmatrix} 0 & S_{12} & 0 \\ S_{21} & 0 & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

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

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

TETRAGONAL SYSTEM

$$T_1 = \begin{pmatrix} S_{11} & -S_{21} & 0 \\ S_{21} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

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}
T_1^a	n_1	n_2	n_3
T_1^b	n_1	n_2	$4n_3 + 1$
T_1^c	n_1	n_2	$4n_3 + 3$
T_1^d	n_1	n_2	$2n_3 + 1$
T_1^e	$2n_1 + 1$	$2n_2$	$2n_3 + 1$
T_1^f	$2n_1$	$2n_2 + 1$	$2n_3 + 1$
T_1^g	$2n_1 + 1$	$2n_2 + 1$	$2n_3$
T_1^h	$2n_1$	$2n_2$	$2n_3$
T_1^i	$2n_1 + 1$	$2n_2$	n_3
T_1^j	$2n_1$	$2n_2 + 1$	n_3

$$T_2 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

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

	S_{11}		S_{33}
T_2^a	n_1		n_2
T_2^b	$2n_1 + 1$		n_2
T_2^c	n_1		$4n_2 + 1$
T_2^d	n_1		$4n_2 + 3$
T_2^e	$2n_1 + 1$		$4n_2 + 1$
T_2^f	$2n_1 + 1$		$4n_2 + 3$
T_2^g	n_1		$2n_2 + 1$
T_2^h	$2n_1 + 1$		$2n_2 + 1$
T_2^i	$2n_1$		$2n_2$

$$T_3 = \begin{pmatrix} S_{11} & -S_{11} & 0 \\ S_{11} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$$

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

$T_3^a : S_{33} = n_1$; $T_3^b : S_{33} = 4n_1 + 1$; $T_3^c : S_{33} = 4n_1 + 1$;
$T_3^d : S_{33} = 2n_1 + 1$; $T_3^e : S_{33} = 2n_1$

The following general rule exists: only those matrices 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 O_1 and 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 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 S [equation (13.1.1.3)] requires the use of special techniques (*cf.* Chapter 13.2, *Derivative lattices*); they apply also to $P\bar{1}$.

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 $t_{\mathcal{G}}$ and the nature of the symmetry operations by means of the column matrices w and w'. The three factors, origin, lattice type, screw and glide components, impose parity conditions on the coefficients of the matrix S. Only a few examples are given here.

When (W, w) and (W', w') are operators of lattice translations of $\mathcal{H}$, say $(I, t_{\mathcal{G}})$ and $(I, t_{\mathcal{H}})$, equation (13.1.1.2*b*) reduces to

$$S \cdot t_{\mathcal{H}} = t_{\mathcal{G}}. \qquad (13.1.1.4)$$

Example

In a tetragonal *I* lattice, $t_{\mathcal{G}}$ is either an integral or a fractional translation. If $t_{\mathcal{H}}$ is $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and the matrix S is replaced by T_1, one obtains

references