

## 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  $\mathbf{a}, \mathbf{b}, \mathbf{c}$  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

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

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

The index of  $\mathcal{H}$  in  $\mathcal{G}$  is equal to  $|\det(\mathbf{S})|$ , which is the ratio of the volumes  $[\mathbf{a}'\mathbf{b}'\mathbf{c}']$  and  $[\mathbf{a}\mathbf{b}\mathbf{c}]$  of the two cells.  $\det(\mathbf{S})$  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  $s$ . Thus, the coordinate system  $(O', \mathbf{a}', \mathbf{b}', \mathbf{c}')$  will be specified completely by the square matrix  $\mathbf{S}$  and the column matrix  $s$ , symbolized by  $\mathbb{S} : (\mathbf{S}, s)$ .

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

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

(*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:

$$\mathbf{S}\mathbf{W}' = \mathbf{W}\mathbf{S}, \quad (13.1.1.2a)$$

$$s + \mathbf{S}\mathbf{w}' = \mathbf{w} + \mathbf{W}s = \hat{\mathbf{w}} + \mathbf{t}_G + \mathbf{W}s$$

or

$$\mathbf{S}\mathbf{w}' - \hat{\mathbf{w}} + (\mathbf{I} - \mathbf{W})s = \mathbf{t}_G. \quad (13.1.1.2b)$$

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

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

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

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  $\mathbf{c}$ ). We also include here the monoclinic system (unique axis either  $c$  or  $b$ ).

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

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

*Monoclinic system*

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

or if  $b$  instead of  $c$  is used

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

*Tetragonal system*

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

*Hexagonal and trigonal systems*

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

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

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

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

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

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

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

### 13.1. ISOMORPHIC SUBGROUPS

Table 13.1.2.1. *Isomorphic subgroups of the plane groups*

#### OBLIQUE SYSTEM

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

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

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

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

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

#### SQUARE SYSTEM

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

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

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

Conditions:  $T_2^a : S_{11} > 1; T_2^b : S_{11} = 2n_1 + 1 > 1$

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

Condition:  $S_{11} > 0$

#### HEXAGONAL SYSTEM

$$H_1 = \begin{pmatrix} S_{11} & -S_{21} \\ S_{21} & S_{11} - S_{21} \end{pmatrix}$$

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

$$H_2 = \begin{pmatrix} S_{11} & 0 \\ 0 & S_{11} \end{pmatrix}$$

Condition:  $S_{11} > 1$

$$H_3 = \begin{pmatrix} 2S_{11} & -S_{11} \\ S_{11} & S_{11} \end{pmatrix}$$

Condition:  $S_{11} > 0$

#### Table of plane subgroups

No. 1 $p1 : S$ ; No. 2 $p2 : S$ ; No. 3 $pm : O^a$ ; No. 4 $pg : O^b$ ;
No. 5 $cm : O^c, O^d$ ; No. 6 $p2mm : O^a$ ; No. 7 $p2mg : O^e$ ; No. 8 $p2gg : O^f$ ;
No. 9 $c2mm : O^c, O^d$ ; No. 10 $p4 : T_1$ ; No. 11 $p4mm : T_2^a, T_3$ ;
No. 12 $p4gm : T_2^b$ ; No. 13 $p3 : H_1$ ; No. 14 $p3m1 : H_2$ ; No. 15 $p31m : H_2$ ;
No. 16 $p6 : H_1$ ; No. 17 $p6mm : H_2, H_3$ .

#### 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  $M_c$  and  $M_b$  apply without any further restrictions on the coefficients.

#### Tetragonal system

The matrix  $T_1$  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 (13.1.1.2a):

(i) If the last two letters of the Hermann–Mauguin symbol are different,  $S_{21} = 0$ ; the corresponding matrix is called  $T_2$ .

Example:  $P4_2/mmc$

$$T_2 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(T_2) = S_{33}S_{11}^2.$$

(ii) If the last two letters are the same (except for the three cases mentioned below), two matrices have to be applied, the matrix  $T_2$  introduced above and the matrix  $T_1$  with  $S_{21} = S_{11}$ ; the corresponding matrix is called  $T_3$ .

$$T_3 = \begin{pmatrix} S_{11} & -S_{11} & 0 \\ S_{11} & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(T_3) = 2S_{33}S_{11}^2.$$

The following space groups have matrices  $T_2$  and  $T_3$ :  $P422, P4mm, P4/mmm, P4_122, P4_322, P4_222, P4cc, P4/mcc, I422, I4mm$  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  $T_2$ .

#### Hexagonal and trigonal systems

The matrix  $H_1$  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  $H_2$ . Examples are  $P6_3/mcm, P312$  and  $P\bar{6}2m$ .

$$H_2 = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(H_2) = S_{33}S_{11}^2.$$

If the last two letters of the Hermann–Mauguin symbol are the same, two matrices have to be applied, the matrix  $H_2$  introduced above and the matrix  $H_1$  with  $S_{11} = 2S'_{11}$  and  $S_{21} = S'_{11}$ ; this matrix is called  $H_3$ ,

$$H_3 = \begin{pmatrix} 2S'_{11} & -S'_{11} & 0 \\ S'_{11} & S'_{11} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}, \quad \det(H_3) = 3S_{33}S_{11}'^2.$$

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

#### Rhombohedral space groups

For  $R3$  and  $R\bar{3}$ , one has the matrix  $H_1$  for hexagonal axes and  $R_1$  for rhombohedral axes. For all other rhombohedral space groups, one has  $H_2$  (hexagonal axes) and the matrix  $R_1$  with  $S_1 = S_2$  (rhombohedral axes). This last matrix is called  $R_2$ . Example:  $R32$ .

### 13. ISOMORPHIC SUBGROUPS OF SPACE GROUPS

Table 13.1.2.2. *Isomorphic subgroups of the space groups*

#### TRICLINIC SYSTEM

$\mathbf{S} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{pmatrix}$
Conditions: $S_{11} > 0, S_{22} > 0, S_{33} > 0, S_{11}S_{22}S_{33} > 1,$ $S_{21} = S_{31} = S_{32} = 0, -S_{11}/2 < S_{12} \leq S_{11}/2,$ $-S_{11}/2 < S_{13} \leq S_{11}/2, -S_{22}/2 < S_{23} \leq S_{22}/2$

#### MONOCLINIC SYSTEM

Unique axis $c$						
$\mathbf{M}_c = \begin{pmatrix} S_{11} & S_{12} & 0 \\ S_{21} & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}$						
Conditions: $S_{33} > 0, (S_{11}S_{22} - S_{12}S_{21})S_{33} > 1$						
	S <sub>11</sub>	S <sub>12</sub>	S <sub>21</sub>	S <sub>22</sub>	S <sub>33</sub>	Extra condition
$M_c^a$	$n_1 > 0$	0	$n_3$	$n_4 > 0$	$n_5$	$-n_4/2 < n_3 \leq n_4/2$
$M_c^b$	$n_1 > 0$	0	$n_3$	$n_4 > 0$	$2n_5 + 1$	$-n_4/2 < n_3 \leq n_4/2$
$M_c^c$	$n_1 > 0$	$2n_2$	0	$2n_4 + 1 > 0$	$2n_5 + 1$	$-n_1/2 < n_2 \leq n_1/2$
$M_c^d$	$n_1 > 0$	$2n_2$	0	$2n_4 > 0$	$2n_5$	$-n_1/2 < n_2 \leq n_1/2$
$M_c^e$	$n_1$	$2n_2 > 0$	$n_3 < 0$	0	$2n_5$	$-n_2 < n_1 \leq n_2$
$M_c^f$	$2n_1 + 1 > 0$	0	$2n_3$	$n_4 > 0$	$n_5$	$-n_4/2 < n_3 \leq n_4/2$
$M_c^g$	$2n_1 + 1 > 0$	$2n_2$	0	$2n_4 + 1 > 0$	$2n_5 + 1$	$-(2n_1 + 1)/2 < n_2 \leq (2n_1 + 1)/2$
$M_c^h$	$2n_1 + 1 > 0$	$2n_2$	0	$2n_4 > 0$	$2n_5$	$-(2n_1 + 1)/2 < n_2 \leq (2n_1 + 1)/2$
$M_c^i$	$2n_1 + 1$	$2n_2 > 0$	$n_3 < 0$	0	$2n_5$	$-(n_2 + 1)/2 < n_1 \leq (n_2 - 1)/2$
$M_c^j$	$2n_1 + 1 > 0$	0	$2n_3$	$n_4 > 0$	$2n_5 + 1$	$-n_4/2 < n_3 \leq n_4/2$
Unique axis $b$						
$\mathbf{M}_b = \begin{pmatrix} S_{11} & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & S_{33} \end{pmatrix}$						
Conditions: $S_{22} > 0, (S_{11}S_{33} - S_{13}S_{31})S_{22} > 1$						
	S <sub>11</sub>	S <sub>13</sub>	S <sub>22</sub>	S <sub>31</sub>	S <sub>33</sub>	Extra condition
$M_b^a$	$n_1 > 0$	$n_2$	$n_3$	0	$n_5 > 0$	$-n_1/2 < n_2 \leq n_1/2$
$M_b^b$	$n_1 > 0$	$n_2$	$2n_3 + 1$	0	$n_5 > 0$	$-n_1/2 < n_2 \leq n_1/2$
$M_b^c$	$2n_1 + 1 > 0$	0	$2n_3 + 1$	$2n_4$	$n_5 > 0$	$-n_5/2 < n_4 \leq n_5/2$
$M_b^d$	$2n_1 > 0$	0	$2n_3$	$2n_4$	$n_5 > 0$	$-n_5/2 < n_4 \leq n_5/2$
$M_b^e$	0	$n_2 < 0$	$2n_3$	$2n_4 > 0$	$n_5$	$-n_4 < n_5 \leq n_4$
$M_b^f$	$n_1$	$2n_2$	$n_3$	0	$2n_5 + 1 > 0$	$-n_1/2 < n_2 \leq n_1/2$
$M_b^g$	$2n_1 + 1 > 0$	0	$2n_3 + 1$	$2n_4$	$2n_5 + 1 > 0$	$-(2n_5 + 1)/2 < n_4 \leq (2n_5 + 1)/2$
$M_b^h$	$2n_1 > 0$	0	$2n_3$	$2n_4$	$2n_5 + 1 > 0$	$-(2n_5 + 1)/2 < n_4 \leq (2n_5 + 1)/2$
$M_b^i$	0	$n_2 < 0$	$2n_3$	$2n_4 > 0$	$2n_5 + 1$	$-(n_4 + 1)/2 < n_5 \leq (n_4 - 1)/2$
$M_b^j$	$n_1 > 0$	$2n_2$	$2n_3 + 1$	0	$2n_5 + 1 > 0$	$-n_1/2 < n_2 \leq n_1/2$

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

#### 13.1.2.2. Cubic and orthorhombic systems

##### Cubic system

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

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

##### Orthorhombic system

There are six choices of matrices  $\mathbf{O}_i$  ( $i = 1, 2, 3, 4, 5, 6$ ) corresponding to the identical orientation ( $\mathbf{O}_1$ ), to cyclic permutations of the three axes ( $\mathbf{O}_2$  and  $\mathbf{O}_3$ ) and to the interchange of two

axes ( $\mathbf{O}_4, \mathbf{O}_5$  and  $\mathbf{O}_6$ ), i.e. to the six orthorhombic 'settings'.

$$\begin{aligned} \mathbf{O}_1 &= \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}; & \mathbf{O}_2 &= \begin{pmatrix} 0 & S_{12} & 0 \\ 0 & 0 & S_{23} \\ S_{31} & 0 & 0 \end{pmatrix}; \\ \mathbf{O}_3 &= \begin{pmatrix} 0 & 0 & S_{13} \\ S_{21} & 0 & 0 \\ 0 & S_{32} & 0 \end{pmatrix}; & \mathbf{O}_4 &= \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & 0 & S_{23} \\ 0 & S_{32} & 0 \end{pmatrix}; \\ \mathbf{O}_5 &= \begin{pmatrix} 0 & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{31} & 0 & 0 \end{pmatrix}; & \mathbf{O}_6 &= \begin{pmatrix} 0 & S_{12} & 0 \\ S_{21} & 0 & 0 \\ 0 & 0 & S_{33} \end{pmatrix}. \end{aligned}$$

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