International Tables for Crystallography (2006). Vol. A, Section 13.1.1.1, p. 836.

13.1. Isomorphic subgroups

BY Y. BILLIET AND E. F. BERTAUT

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.

Copyright © 2006 International Union of Crystallography

references