

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

Table 1.4.2.6

Right coset decomposition of space group $P2_1/c$, No. 14 (unique axis b , cell choice 1) with respect to the normal subgroup of translations \mathcal{T}

The numbers u_1, u_2 and u_3 are positive or negative integers.

| | | | | | | | | | | | |
|-----------|-----------|-----------|-----------------|-------------------------|-------------------------------|-----------------|-----------------|-----------------|-----------|-------------------------------|-------------------------|
| x | y | z | \bar{x} | $y + \frac{1}{2}$ | $\bar{z} + \frac{1}{2}$ | \bar{x} | \bar{y} | \bar{z} | x | $\bar{y} + \frac{1}{2}$ | $z + \frac{1}{2}$ |
| $x + 1$ | y | z | $\bar{x} + 1$ | $y + \frac{1}{2}$ | $\bar{z} + \frac{1}{2}$ | $\bar{x} + 1$ | \bar{y} | \bar{z} | $x + 1$ | $\bar{y} + \frac{1}{2}$ | $z + \frac{1}{2}$ |
| $x + 2$ | y | z | $\bar{x} + 2$ | $y + \frac{1}{2}$ | $\bar{z} + \frac{1}{2}$ | $\bar{x} + 2$ | \bar{y} | \bar{z} | $x + 2$ | $\bar{y} + \frac{1}{2}$ | $z + \frac{1}{2}$ |
| \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots |
| x | $y + 1$ | z | \bar{x} | $y + \frac{3}{2}$ | $\bar{z} + \frac{1}{2}$ | \bar{x} | $\bar{y} + 1$ | \bar{z} | x | $\bar{y} + \frac{3}{2}$ | $z + \frac{1}{2}$ |
| $x + 1$ | $y + 1$ | z | $\bar{x} + 1$ | $y + \frac{3}{2}$ | $\bar{z} + \frac{1}{2}$ | $\bar{x} + 1$ | $\bar{y} + 1$ | \bar{z} | $x + 1$ | $\bar{y} + \frac{3}{2}$ | $z + \frac{1}{2}$ |
| $x + 2$ | $y + 1$ | z | $\bar{x} + 2$ | $y + \frac{3}{2}$ | $\bar{z} + \frac{1}{2}$ | $\bar{x} + 2$ | $\bar{y} + 1$ | \bar{z} | $x + 2$ | $\bar{y} + \frac{3}{2}$ | $z + \frac{1}{2}$ |
| \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots |
| x | $y + 2$ | z | \bar{x} | $y + \frac{5}{2}$ | $\bar{z} + \frac{1}{2}$ | \bar{x} | $\bar{y} + 2$ | \bar{z} | x | $\bar{y} + \frac{5}{2}$ | $z + \frac{1}{2}$ |
| $x + 1$ | $y + 2$ | z | $\bar{x} + 1$ | $y + \frac{5}{2}$ | $\bar{z} + \frac{1}{2}$ | $\bar{x} + 1$ | $\bar{y} + 2$ | \bar{z} | $x + 1$ | $\bar{y} + \frac{5}{2}$ | $z + \frac{1}{2}$ |
| $x + 2$ | $y + 2$ | z | $\bar{x} + 2$ | $y + \frac{5}{2}$ | $\bar{z} + \frac{1}{2}$ | $\bar{x} + 2$ | $\bar{y} + 2$ | \bar{z} | $x + 2$ | $\bar{y} + \frac{5}{2}$ | $z + \frac{1}{2}$ |
| \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots |
| x | y | $z + 1$ | \bar{x} | $y + \frac{1}{2}$ | $\bar{z} + \frac{3}{2}$ | \bar{x} | \bar{y} | $\bar{z} + 1$ | x | $\bar{y} + \frac{1}{2}$ | $z + \frac{3}{2}$ |
| $x + 1$ | y | $z + 1$ | $\bar{x} + 1$ | $y + \frac{1}{2}$ | $\bar{z} + \frac{3}{2}$ | $\bar{x} + 1$ | \bar{y} | $\bar{z} + 1$ | $x + 1$ | $\bar{y} + \frac{1}{2}$ | $z + \frac{3}{2}$ |
| $x + 2$ | y | $z + 1$ | $\bar{x} + 2$ | $y + \frac{1}{2}$ | $\bar{z} + \frac{3}{2}$ | $\bar{x} + 2$ | \bar{y} | $\bar{z} + 1$ | $x + 2$ | $\bar{y} + \frac{1}{2}$ | $z + \frac{3}{2}$ |
| \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots |
| x | $y + 1$ | $z + 1$ | \bar{x} | $y + \frac{3}{2}$ | $\bar{z} + \frac{3}{2}$ | \bar{x} | $\bar{y} + 1$ | $\bar{z} + 1$ | x | $\bar{y} + \frac{3}{2}$ | $z + \frac{3}{2}$ |
| $x + 1$ | $y + 1$ | $z + 1$ | $\bar{x} + 1$ | $y + \frac{3}{2}$ | $\bar{z} + \frac{3}{2}$ | $\bar{x} + 1$ | $\bar{y} + 1$ | $\bar{z} + 1$ | $x + 1$ | $\bar{y} + \frac{3}{2}$ | $z + \frac{3}{2}$ |
| $x + 2$ | $y + 1$ | $z + 1$ | $\bar{x} + 2$ | $y + \frac{3}{2}$ | $\bar{z} + \frac{3}{2}$ | $\bar{x} + 2$ | $\bar{y} + 1$ | $\bar{z} + 1$ | $x + 2$ | $\bar{y} + \frac{3}{2}$ | $z + \frac{3}{2}$ |
| \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots |
| $x + u_1$ | $y + u_2$ | $z + u_3$ | $\bar{x} + u_1$ | $y + u_2 + \frac{1}{2}$ | $\bar{z} + u_3 + \frac{1}{2}$ | $\bar{x} + u_1$ | $\bar{y} + u_2$ | $\bar{z} + u_3$ | $x + u_1$ | $\bar{y} + u_2 + \frac{1}{2}$ | $z + u_3 + \frac{1}{2}$ |
| \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots | \vdots |

set of matrix–column pairs $\{(\mathbf{W}, \mathbf{w})\}$. The set $\mathcal{T}_G = \{(\mathbf{I}, \mathbf{t})\}$ of all translations forms the *translation subgroup* $\mathcal{T}_G \triangleleft \mathcal{G}$, which is a normal subgroup of \mathcal{G} of finite index $[i]$. If (\mathbf{W}, \mathbf{w}) is a fixed symmetry operation, then all the products $\mathcal{T}_G(\mathbf{W}, \mathbf{w}) = \{(\mathbf{I}, \mathbf{t})(\mathbf{W}, \mathbf{w}) = \{(\mathbf{W}, \mathbf{w} + \mathbf{t})\}$ of translations with (\mathbf{W}, \mathbf{w}) have the same rotation part \mathbf{W} . Conversely, every symmetry operation \mathbf{W} of \mathcal{G} with the same matrix part \mathbf{W} is represented in the set $\mathcal{T}_G(\mathbf{W}, \mathbf{w})$. The infinite set of symmetry operations $\mathcal{T}_G(\mathbf{W}, \mathbf{w})$ is called a coset of the right coset decomposition of \mathcal{G} with respect to \mathcal{T}_G , and (\mathbf{W}, \mathbf{w}) its coset representative. In this way, the symmetry operations of \mathcal{G} can be distributed into a finite set of infinite cosets, the elements of which are obtained by the combination of a coset representative $(\mathbf{W}_j, \mathbf{w}_j)$ and the infinite set $\mathcal{T}_G = \{(\mathbf{I}, \mathbf{t})\}$ of translations (cf. Section 1.3.3.2):

$$\mathcal{G} = \mathcal{T}_G \cup \mathcal{T}_G(\mathbf{W}_2, \mathbf{w}_2) \cup \dots \cup \mathcal{T}_G(\mathbf{W}_m, \mathbf{w}_m) \cup \dots \cup \mathcal{T}_G(\mathbf{W}_i, \mathbf{w}_i), \tag{1.4.2.1}$$

where $(\mathbf{W}_1, \mathbf{w}_1) = (\mathbf{I}, \mathbf{o})$ is omitted. Obviously, the coset representatives $(\mathbf{W}_j, \mathbf{w}_j)$ of the decomposition $(\mathcal{G} : \mathcal{T}_G)$ represent in a clear and compact way the infinite number of symmetry operations of the space group \mathcal{G} . Each coset in the decomposition $(\mathcal{G} : \mathcal{T}_G)$ is characterized by its linear part \mathbf{W}_j and its entries differ only by lattice translations. The translations $(\mathbf{I}, \mathbf{t}) \in \mathcal{T}_G$ form the first coset with the identity (\mathbf{I}, \mathbf{o}) as a coset representative. The symmetry operations with rotation part \mathbf{W}_2 form the second coset etc. The number of cosets equals the number of different matrices \mathbf{W}_j of the symmetry operations of the space group. This number $[i]$ is always finite and is equal to the order of the point group \mathcal{P}_G of the space group (cf. Section 1.3.3.2).

For each space group, a set of coset representatives $\{(\mathbf{W}_j, \mathbf{w}_j), 1 \leq j \leq [i]\}$ of the decomposition $(\mathcal{G} : \mathcal{T}_G)$ is listed under the general-position block of the space-group tables. In general, any element of a coset may be chosen as a coset representative. For convenience, the representatives listed in the space-group tables are always chosen such that the components $w_{j,k}, k = 1, 2, 3$, of the translation parts \mathbf{w}_j fulfil $0 \leq w_{j,k} < 1$ (by

subtracting integers). To save space, each matrix–column pair $(\mathbf{W}_j, \mathbf{w}_j)$ is represented by the corresponding *coordinate triplet* (cf. Section 1.2.2.3 for the shorthand notation of matrix–column pairs).

Example

The right coset decomposition of $P2_1/c$, No. 14 (unique axis b , cell choice 1) with respect to its translation subgroup is shown in Table 1.4.2.6. All possible symmetry operations of $P2_1/c$ are distributed into four cosets:

The first column represents the infinitely many translations $t = (\mathbf{I}, \mathbf{t}) = x + u_1, y + u_2, z + u_3 = \{1|u_1, u_2, u_3\}$ of the translation subgroup \mathcal{T} of $P2_1/c$. The numbers u_1, u_2 and u_3 are positive or negative integers. The identity operation (\mathbf{I}, \mathbf{o}) is usually chosen as a coset representative.

The third coset of the decomposition $(\mathcal{G} : \mathcal{T}_G)$ represents the infinite set of inversions $(-\mathbf{I}, \mathbf{t}) = \bar{x} + u_1, \bar{y} + u_2, \bar{z} + u_3 = \{\bar{1}|u_1, u_2, u_3\}$ of the space group $P2_1/c$ with inversion centres located at $u_1/2, u_2/2, u_3/2$ (cf. Section 1.2.2.4 for the determination of the location of the inversion centres). The inversion in the origin, i.e. $\bar{x}, \bar{y}, \bar{z} = \{\bar{1}|0\}$, is taken as a coset representative.

The coset representative of the second coset is the twofold screw rotation $\{2_{010}|0, \frac{1}{2}, \frac{1}{2}\}$ around the line $0, y, \frac{1}{4}$, followed by its infinite combinations with all lattice translations: $\bar{x} + u_1, y + \frac{1}{2} + u_2, \bar{z} + \frac{1}{2} + u_3 = \{2_{010}|u_1, \frac{1}{2} + u_2, \frac{1}{2} + u_3\}$. These are twofold screw rotations around the lines $u_1/2, y, u_3/2 + \frac{1}{4}$ with

screw components $\begin{pmatrix} 0 \\ \frac{1}{2} + u_2 \\ 0 \end{pmatrix}$.

The symmetry operations of the fourth column represented by $x + u_1, \bar{y} + \frac{1}{2} + u_2, z + \frac{1}{2} + u_3 = \{m_{010}|u_1, \frac{1}{2} + u_2, \frac{1}{2} + u_3\}$ correspond to glide reflections with glide components

$\begin{pmatrix} u_1 \\ 0 \\ \frac{1}{2} + u_3 \end{pmatrix}$ through the (infinite) set of glide planes at $x, \frac{1}{4}, z$;