Table 1.3.3.2
Automorphism groups of three-dimensional primitive lattices

Lattice	Metric tensor	Bravais group	
		Hermann–Mauguin symbol	Generators
Triclinic	$\begin{pmatrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{pmatrix}$	$\bar{1}$	$\bar{1}$: $\bar{x}, \bar{y}, \bar{z}$
Monoclinic	$\begin{pmatrix} g_{11} & 0 & g_{13} \\ & g_{22} & 0 \\ & & g_{33} \end{pmatrix}$	$2/m$	2_{010}: $\bar{x}, y, \bar{z}$ m_{010}: $x, \bar{y}, z$
Orthorhombic	$\begin{pmatrix} g_{11} & 0 & 0 \\ & g_{22} & 0 \\ & & g_{33} \end{pmatrix}$	mmm	m_{100}: $\bar{x}, y, z$ m_{010}: $x, \bar{y}, z$ m_{001}: $x, y, \bar{z}$
Tetragonal	$\begin{pmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{pmatrix}$	$4/mmm$	4_{001}: $\bar{y}, x, z$ m_{001}: $x, y, \bar{z}$ m_{100}: $\bar{x}, y, z$
Hexagonal	$\begin{pmatrix} g_{11} & -\frac{1}{2}g_{11} & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{pmatrix}$	$6/mmm$	6_{001}: $x-y, x, z$ m_{001}: $x, y, \bar{z}$ m_{100}: $\bar{x}+y, y, z$
Rhombohedral	$\begin{pmatrix} g_{11} & g_{12} & g_{12} \\ & g_{11} & g_{12} \\ & & g_{11} \end{pmatrix}$	$\bar{3}m$	$\bar{3}_{111}$: $\bar{z}, \bar{x}, \bar{y}$ $m_{1\bar{1}0}$: y, x, z
Cubic	$\begin{pmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{pmatrix}$	$m\bar{3}m$	m_{001}: $x, y, \bar{z}$ $\bar{3}_{111}$: $\bar{z}, \bar{x}, \bar{y}$ m_{110}: $\bar{y}, \bar{x}, z$

Table 1.3.3.3
Right-coset decomposition of $\mathcal{G}$ relative to $\mathcal{T}$

$W_1 = e$	W_2	W_3	...	$W_{[i]}$
t_1	t_1W_2	t_1W_3	...	$t_1W_{[i]}$
t_2	t_2W_2	t_2W_3	...	$t_2W_{[i]}$
t_3	t_3W_2	t_3W_3	...	$t_3W_{[i]}$
t_4	t_4W_2	t_4W_3	...	$t_4W_{[i]}$
$\vdots$	$\vdots$	$\vdots$		$\vdots$

Remark: We can assume some enumeration $t_1, t_2, t_3, \ldots$ of the operations in $\mathcal{T}$ because the translation vectors form a lattice. For example, with respect to a primitive basis, the coordinate vectors of the translations in $\mathcal{G}$ are simply columns $\begin{pmatrix} l \\ m \\ n \end{pmatrix}$ with integral components l, m, n. A straightforward enumeration of these columns would start with

$$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} \bar{1} \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \bar{1} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \bar{1} \end{pmatrix},$$
$$\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \ldots$$

Writing out the matrix–column pairs, the coset $\mathcal{T}(\boldsymbol{W}, \boldsymbol{w})$ consists of the operations of the form $(\boldsymbol{I}, \boldsymbol{t})(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w} + \boldsymbol{t})$ with $\boldsymbol{t}$ running over the lattice translations of $\mathcal{T}$. This means that the operations of a coset with respect to the translation subgroup all have the same linear part, which is also evident from a listing of the cosets as columns of an infinite array, as in the example above.

Proposition

Let $W = (\boldsymbol{W}, \boldsymbol{w})$ and $W' = (\boldsymbol{W}', \boldsymbol{w}')$ be two operations of a space group $\mathcal{G}$ with translation subgroup $\mathcal{T}$.

(1) If $\boldsymbol{W} \neq \boldsymbol{W}'$, then the cosets $\mathcal{T}W$ and $\mathcal{T}W'$ are disjoint, *i.e.* their intersection is empty.

(2) If $\boldsymbol{W} = \boldsymbol{W}'$, then the cosets $\mathcal{T}W$ and $\mathcal{T}W'$ are equal, because WW'^{-1} has linear part $\boldsymbol{I}$ and is thus an operation contained in $\mathcal{T}$.

The one-to-one correspondence between the point-group operations and the cosets relative to $\mathcal{T}$ explicitly displays the isomorphism between the point group $\mathcal{P}$ of $\mathcal{G}$ and the factor group $\mathcal{G}/\mathcal{T}$. This correspondence is also exploited in the listing of the general-position coordinates. What is given there are the coordinate triplets for coset representatives of $\mathcal{G}$ relative to $\mathcal{T}$, which correspond to the first row of the array in Table 1.3.3.3. As just explained, the other operations in $\mathcal{G}$ can be obtained from these coset representatives by adding a lattice translation to the translational part.

Furthermore, the correspondence between the point group and the coset decomposition relative to $\mathcal{T}$ makes it easy to find a system of coset representatives $\{W_1, \ldots, W_m\}$ of $\mathcal{G}$ relative to $\mathcal{T}$. What is required is that the linear parts of the W_i are precisely the operations in the point group of $\mathcal{G}$. If $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_m$ are the different operations in the point group $\mathcal{P}$ of $\mathcal{G}$, then a system of coset representatives is obtained by choosing for every linear part $\boldsymbol{W}_i$ a translation part $\boldsymbol{w}_i$ such that $W_i = (\boldsymbol{W}_i, \boldsymbol{w}_i)$ is an operation in $\mathcal{G}$.

It is customary to choose the translation parts $\boldsymbol{w}_i$ of the coset representatives such that their coordinates lie between 0 and 1,

references