

1. GENERAL RELATIONSHIPS AND TECHNIQUES

Table A1.4.2.2. Lattice symbol L

The lattice symbol L implies Seitz matrices for the lattice translations. For noncentrosymmetric lattices the rotation parts of the Seitz matrices are for I (see Table A1.4.2.4). For centrosymmetric lattices the rotation parts are I and $-I$. The translation parts in the fourth columns of the Seitz matrices are listed in the last column of the table. The total number of matrices implied by each symbol is given by nS .

Noncentrosymmetric		Centrosymmetric		
Symbol	nS	Symbol	nS	Implied lattice translation(s)
P	1	$-P$	2	0, 0, 0
A	2	$-A$	4	0, 0, 0 0, $\frac{1}{2}$, $\frac{1}{2}$
B	2	$-B$	4	0, 0, 0 $\frac{1}{2}$, 0, $\frac{1}{2}$
C	2	$-C$	4	0, 0, 0 $\frac{1}{2}$, $\frac{1}{2}$, 0
I	2	$-I$	4	0, 0, 0 $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$
R	3	$-R$	6	0, 0, 0 $\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{3}$ $\frac{1}{3}$, $\frac{2}{3}$, $\frac{2}{3}$
H	3	$-H$	6	0, 0, 0 $\frac{2}{3}$, $\frac{1}{3}$, 0 $\frac{1}{3}$, $\frac{2}{3}$, 0
F	4	$-F$	8	0, 0, 0 0, $\frac{1}{2}$, $\frac{1}{2}$ $\frac{1}{2}$, 0, $\frac{1}{2}$ $\frac{1}{2}$, $\frac{1}{2}$, 0

$$\left[\begin{pmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \right] = \begin{pmatrix} \bar{z} \\ \bar{x} \\ \bar{y} \end{pmatrix},$$

$$\left[\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} \frac{1}{4} \\ \frac{3}{4} \\ \frac{1}{4} \end{pmatrix} \right] = \begin{pmatrix} \frac{1}{4} - y \\ \frac{3}{4} + x \\ \frac{1}{4} + z \end{pmatrix},$$

$$\left[\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} \frac{3}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix} \right] = \begin{pmatrix} \frac{3}{4} + y \\ \frac{1}{4} + x \\ \frac{1}{4} - z \end{pmatrix}.$$

The corresponding symmetry transformations in reciprocal space, in the notation of Section 1.4.4, are

$$\left[(hkl) \begin{pmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix} : -(hkl) \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \right] = [\bar{k}\bar{l}h : 0];$$

similarly, $[\bar{k}\bar{l}h : -131/4]$ and $[k\bar{l}h : -311/4]$ are obtained from the second and third generator of $Ia\bar{3}d$, respectively.

The first column of Table A1.4.2.1 lists the conventional space-group number. The second column shows the conventional short Hermann–Mauguin or international space-group symbol, and the third column, *Comments*, shows the full international space-group symbol *only* for the different settings of the monoclinic space groups that are given in the main space-group tables of *IT A* (1983). Other comments pertain to the choice of the space-group origin – where there are alternatives – and to axial systems. The fourth column shows the explicit space-group symbols described above for each of the settings considered in *IT A* (1983).

A1.4.2.3. Hall symbols (S. R. HALL AND R. W. GROSSE-KUNSTLEVE)

The explicit-origin space-group notation proposed by Hall (1981a) is based on a subset of the symmetry operations, in the form of Seitz matrices, sufficient to uniquely define a space group. The concise unambiguous nature of this notation makes it well suited to handling symmetry in computing and database applications.

Table A1.4.2.7 lists space-group notation in several formats. The first column of Table A1.4.2.7 lists the space-group numbers with axis codes appended to identify the non-standard settings. The second column lists the Hermann–Mauguin symbols in computer-entry format with appended codes to identify the origin and cell choice when there are alternatives. The general forms of the Hall notation are listed in the fourth column and the computer-entry representations of these symbols are listed in the third column. The computer-entry format is the general notation expressed as case-insensitive ASCII characters with the overline (bar) symbol replaced by a minus sign.

The Hall notation has the general form:

$$L[N_T^A]_1 \dots [N_T^A]_p V. \quad (\text{A1.4.2.4})$$

L is the symbol specifying the lattice translational symmetry (see Table A1.4.2.2). The integral translations are implicitly included in the set of generators. If L has a leading minus sign, it also specifies an inversion centre at the origin. $[N_T^A]_n$ specifies the 4×4 Seitz matrix S_n of a symmetry element in the minimum set which defines the space-group symmetry (see Tables A1.4.2.3 to A1.4.2.6), and p is the number of elements in the set. V is a change-of-basis operator needed for less common descriptions of the space-group symmetry.

Table A1.4.2.3. Translation symbol T

The symbol T specifies the translation elements of a Seitz matrix. Alphabetical symbols (given in the first column) specify translations along a fixed direction. Numerical symbols (given in the third column) specify translations as a fraction of the rotation order $|N|$ and in the direction of the implied or explicitly defined axis.

Translation symbol	Translation vector	Subscript symbol	Fractional translation
a	$\frac{1}{2}, 0, 0$	1 in 3_1	$\frac{1}{3}$
b	$0, \frac{1}{2}, 0$	2 in 3_2	$\frac{2}{3}$
c	$0, 0, \frac{1}{2}$	1 in 4_1	$\frac{1}{4}$
n	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	3 in 4_3	$\frac{3}{4}$
u	$\frac{1}{4}, 0, 0$	1 in 6_1	$\frac{1}{6}$
v	$0, \frac{1}{4}, 0$	2 in 6_2	$\frac{1}{3}$
w	$0, 0, \frac{1}{4}$	4 in 6_4	$\frac{2}{3}$
d	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	5 in 6_5	$\frac{5}{6}$