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 *1* (see Table A1.4.2.4). For centrosymmetric lattices the rotation parts are *1* and *−1*. 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 $0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$

and (A1.4.2.2)] leads to the new representation of the space group.

In order to illustrate an explicit space-group symbol consider, for example, the symbol for the space group $Ia\bar{3}d$, as given in Table A1.4.2.1:

```
ICC$I3Q000$P4C393$P2D933.
```

The first three characters tell us that the Bravais lattice of this space group is of type `I`, that the space group is centrosymmetric and that it belongs to the cubic system. We then see that the generators are (i) an improper threefold axis along [111] (`I3Q`) with a zero translation part, (ii) a proper fourfold axis along [001] (`P4C`) with translation part (1/4, 3/4, 1/4) and (iii) a proper twofold axis along [110] (`P2D`) with translation part (3/4, 1/4, 1/4).

If we make use of the above-outlined interpretation of the explicit symbol (A1.4.2.3), the space-group symmetry transformations in direct space, corresponding to these three generators of the space group $Ia\bar{3}d$, become

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

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

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

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

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

similarly, $[k\bar{h}l : -131/4]$ and $[kh\bar{l} : -311/4]$ 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

By S. R. Hall and R. W. Grosse-Kunstleve

The explicit-origin space-group notation proposed by Hall (1981*a*) 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 nonstandard 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:

$$\mathbf{L}[\mathbf{N}^{\mathbf{A}}_{\mathbf{T}}]_{\mathbf{1}} \ldots [\mathbf{N}^{\mathbf{A}}_{\mathbf{T}}]_{\mathbf{p}}\mathbf{V}. \qquad \text{(A1.4.2.4)}$$

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	$\frac{5}{6}$

  references