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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	$\frac{5}{6}$

Table A1.4.2.4. *Rotation matrices for principal axes*

The 3×3 matrices for *proper* rotations along the three principal unit-cell directions are given below. The matrices for *improper* rotations (*−1*, *−2*, *−3*, *−4* and *−6*) are identical except that the signs of the elements are reversed.

		Rotation order				
Axis	Symbol A	*1*	*2*	*3*	*4*	*6*
a	*x*	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&\bar{1}&0\\0&0&\bar{1}\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&0&\bar{1}\\0&1&\bar{1}\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&0&\bar{1}\\0&1&0\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&\bar{1}\\0&1&0\end{pmatrix}$
b	*y*	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}\bar{1}&0&0\\0&1&0\\0&0&\bar{1}\end{pmatrix}$	$\begin{pmatrix}\bar{1}&0&1\\0&1&0\\\bar{1}&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\0&1&0\\\bar{1}&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\0&1&0\\\bar{1}&0&1\end{pmatrix}$
c	*z*	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&\bar{1}&0\\1&\bar{1}&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&\bar{1}&0\\1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&\bar{1}&0\\1&0&0\\0&0&1\end{pmatrix}$

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. $[\mathbf{N}^{\mathbf{A}}_{\mathbf{T}}]_{\mathbf{n}}$ specifies the 4×4 Seitz matrix $\mathbf{S_n}$ 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.

The matrix symbol $\mathbf{N}^{\mathbf{A}}_{\mathbf{T}}$ is composed of three parts: **N** is the symbol denoting the |N|-fold order of the rotation matrix (see Tables A1.4.2.4, A1.4.2.5 and A1.4.2.6), **T** is a subscript symbol denoting the *translation* vector (see Table A1.4.2.3) and **A** is a superscript symbol denoting the *axis* of rotation.

The computer-entry format of the Hall notation contains the rotation-order symbol **N** as positive integers *1*, *2*, *3*, *4*, or *6* for proper rotations and as negative integers *−1*, *−2*, *−3*, *−4* or *−6* for improper rotations. The **T** translation symbols *1*, *2*, *3*, *4*, *5*, *6*, *a*, *b*, *c*, *n*, *u*, *v*, *w*, *d* are described in Table A1.4.2.3. These translations apply additively [*e.g.* *ad* signifies a $(\frac{3}{4}, \frac{1}{4}, \frac{1}{4})$ translation]. The **A** axis symbols *x*, *y*, *z* denote rotations about the axes **a**, **b** and **c**, respectively (see Table A1.4.2.4). The axis symbols ″ and ′ signal rotations about the body-diagonal vectors **a** + **b** (or alternatively **b** + **c** or **c** + **a**) and **a** − **b** (or alternatively **b** − **c** or **c** − **a**) (see Table A1.4.2.5). The axis symbol * always refers to a threefold rotation along **a** + **b** + **c** (see Table A1.4.2.6).

Table A1.4.2.5. *Rotation matrices for face-diagonal axes*

The symbols for face-diagonal twofold rotations are *2′* and *2″*. The face-diagonal axis direction is determined by the axis of the preceding rotation N^x, N^y or N^z. Note that the single prime ′ is the default and may be omitted.

Preceding rotation	Rotation	Axis	Matrix
N^x	*2′*	**b** − **c**	$\begin{pmatrix}\bar{1}&0&0\\0&0&\bar{1}\\0&\bar{1}&0\end{pmatrix}$
	2″	**b** + **c**	$\begin{pmatrix}\bar{1}&0&0\\0&0&1\\0&1&0\end{pmatrix}$
N^y	*2′*	**a** − **c**	$\begin{pmatrix}0&0&\bar{1}\\0&\bar{1}&0\\\bar{1}&0&0\end{pmatrix}$
	2″	**a** + **c**	$\begin{pmatrix}0&0&1\\0&\bar{1}&0\\1&0&0\end{pmatrix}$
N^z	*2′*	**a** − **b**	$\begin{pmatrix}0&\bar{1}&0\\\bar{1}&0&0\\0&0&\bar{1}\end{pmatrix}$
	2″	**a** + **b**	$\begin{pmatrix}0&1&0\\1&0&0\\0&0&\bar{1}\end{pmatrix}$

The change-of-basis operator **V** has the general form (v_x, v_y, v_z). The vectors v_x, v_y and v_z are specified by

$$v_x = r_{1,1}X + r_{1,2}Y + r_{1,3}Z + \mathbf{t}_1$$
$$v_y = r_{2,1}X + r_{2,2}Y + r_{2,3}Z + \mathbf{t}_2\,,$$
$$v_z = r_{3,1}X + r_{3,2}Y + r_{3,3}Z + \mathbf{t}_3$$

where $r_{i,j}$ and $\mathbf{t}_i$ are fractions or real numbers. Terms in which $r_{i,j}$ or $\mathbf{t}_i$ are zero need not be specified. The 4×4 change-of-basis matrix operator **V** is defined as

$$\mathbf{V} = \begin{pmatrix} r_{1,1} & r_{1,2} & r_{1,3} & \mathbf{t}_1 \\ r_{2,1} & r_{2,2} & r_{2,3} & \mathbf{t}_2 \\ r_{3,1} & r_{3,2} & r_{3,3} & \mathbf{t}_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The transformed symmetry operations are derived from the specified Seitz matrices $\mathbf{S_n}$ as

$$\mathbf{S}'_{\mathbf{n}} = \mathbf{V} \cdot \mathbf{S_n} \cdot \mathbf{V}^{-1}$$

and from the integral translations **t**(1, 0, 0), **t**(0, 1, 0) and **t**(0, 0, 1) as

$$(\mathbf{t}'_{\mathbf{n}}, \mathbf{1})^T = \mathbf{V} \cdot (\mathbf{t_n}, \mathbf{1})^T.$$

A shorthand form of **V** may be used when the change-of-basis operator only translates the origin of the basis system. In this form v_x, v_y and v_z are specified simply as shifts in twelfths, implying the matrix operator

Table A1.4.2.6. *Rotation matrix for the body-diagonal axis*

The symbol for the threefold rotation in the **a** + **b** + **c** direction is *3**. Note that for cubic space groups the body-diagonal axis is implied and the asterisk * may be omitted.

Axis	Rotation	Matrix
a + **b** + **c**	*3**	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$

$$\mathbf{V} = \begin{pmatrix} 1 & 0 & 0 & v_x/12 \\ 0 & 1 & 0 & v_y/12 \\ 0 & 0 & 1 & v_z/12 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

In the shorthand form of **V**, the commas separating the vectors may be omitted.

A1.4.2.3.1. Default axes

For most symbols the rotation axes applicable to each **N** are implied and an explicit axis symbol **A** is not needed. The rules for *default* axis directions are:

(i) the *first* rotation or roto-inversion has an axis direction of **c**;

(ii) the *second* rotation (if |N| is 2) has an axis direction of **a** if preceded by an |N| of 2 or 4, **a**−**b** if preceded by an |N| of 3 or 6;

(iii) the *third* rotation (if |N| is 3) has an axis direction of **a** + **b** + **c**.

A1.4.2.3.2. Example matrices

The following examples show how the notation expands to Seitz matrices.

The notation $\bar{2}^x_c$ represents an improper twofold rotation along **a** and a **c**/2 translation:

$$-2\text{xc} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The notation 3^* represents a threefold rotation along **a** + **b** + **c**:

$$3^* = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The notation 4_{vw} represents a fourfold rotation along **c** (implied) and translation of **b**/4 and **c**/4:

$$4\text{vw} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & 1 & \frac{1}{4} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The notation 6_1 2 (0 0 −1) represents a 6_1 screw along **c**, a twofold rotation along **a** − **b** and an origin shift of −**c**/12. Note that the 6_1 matrix is unchanged by the shifted origin whereas the *2* matrix is changed by −**c**/6.

$$61\,2\,(0\,0\,{-1}) = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{6} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \frac{5}{6} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The change-of-basis vector (0 0 −1) could also be entered as (x, y, z − 1/12).

The *reverse setting of the R-centred lattice* (hexagonal axes) is specified using a change-of-basis transformation applied to the standard *obverse setting* (see Table A1.4.2.2). The obverse Seitz matrices are

$$\text{R}\,3 = \begin{pmatrix} 1 & 0 & 0 & \frac{1}{3} \\ 0 & 1 & 0 & \frac{2}{3} \\ 0 & 0 & 1 & \frac{2}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & \frac{2}{3} \\ 0 & 1 & 0 & \frac{1}{3} \\ 0 & 0 & 1 & \frac{1}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The reverse-setting Seitz matrices are

$$\text{R}\,3\,(-\text{x}, -\text{y}, \text{z}) = \begin{pmatrix} 1 & 0 & 0 & \frac{1}{3} \\ 0 & 1 & 0 & \frac{2}{3} \\ 0 & 0 & 1 & \frac{1}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & \frac{2}{3} \\ 0 & 1 & 0 & \frac{1}{3} \\ 0 & 0 & 1 & \frac{2}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The conventional primitive hexagonal lattice may be transformed to a *C-centred orthohexagonal setting* using the change-of-basis operator

$$\text{P}\,6\,(\text{x} - 1/2\text{y}, 1/2\text{y}, \text{z}) = \begin{pmatrix} \frac{1}{2} & -\frac{3}{2} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

In this case the lattice translation for the *C* centring is obtained by transforming the integral translation **t**(0, 1, 0):

$$\boldsymbol{V} \cdot \begin{pmatrix} 0 & 1 & 0 & 1 \end{pmatrix}^T = \begin{pmatrix} 1 & -\frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & 0 & 1 \end{pmatrix}^T.$$

The standard setting of an *I*-centred tetragonal space group may be transformed to a primitive setting using the change-of-basis operator

$$\text{I}\,4\,(\text{y} + \text{z}, \text{x} + \text{z}, \text{x} + \text{y}) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Note that in the primitive setting, the fourfold axis is along **a** + **b**.

references