

1. GENERAL RELATIONSHIPS AND TECHNIQUES

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.

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

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. $[\mathbf{N}_T^A]_n$ 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}_T^A is composed of three parts: **N** is the symbol denoting the $|\mathbf{N}|$ -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 $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ 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).

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

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

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

$$\mathbf{S}'_n = \mathbf{V} \cdot \mathbf{S}_n \cdot \mathbf{V}^{-1}$$

and from the integral translations $\mathbf{t}(1, 0, 0)$, $\mathbf{t}(0, 1, 0)$ and $\mathbf{t}(0, 0, 1)$ as

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

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

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	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$