

## 1.4. SYMMETRY IN RECIPROCAL SPACE

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

The  $3 \times 3$  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
<b>a</b>	<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>b</b>	<i>y</i>	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 1 \end{pmatrix}$
<b>c</b>	<i>z</i>	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

The matrix symbol  $N_T^A$  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).

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  $4 \times 4$  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 **S<sub>n</sub>** as

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

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

$$(\mathbf{t}_{\mathbf{n}}, \mathbf{1})^T = \mathbf{V} \cdot (\mathbf{t}_{\mathbf{n}}, \mathbf{1})^T.$$

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
<b>a + b + c</b>	$3^*$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$

Preceding rotation	Rotation	Axis	Matrix
$N^x$	$2'$	<b>b - c</b>	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \end{pmatrix}$
	$2''$	<b>b + c</b>	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$
$N^y$	$2'$	<b>a - c</b>	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$
	$2''$	<b>a + c</b>	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 0 \end{pmatrix}$
$N^z$	$2'$	<b>a - b</b>	$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
	$2''$	<b>a + b</b>	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$