International Tables for Crystallography (2010). Vol. B, Table A1.4.2.6, p. 128.

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	*x*	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&\bar1&0\\0&0&\bar1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&0&\bar1\\0&1&\bar1\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&0&\bar1\\0&1&0\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&1&\bar1\\0&1&0\end{pmatrix}$
b	*y*	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}\bar1&0&0\\0&1&0\\0&0&\bar1\end{pmatrix}$	$\begin{pmatrix}\bar1&0&1\\0&1&0\\\bar1&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\0&1&0\\\bar1&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\0&1&0\\\bar1&0&1\end{pmatrix}$
c	*z*	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}\bar1&0&0\\0&\bar1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&\bar1&0\\1&\bar1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&\bar1&0\\1&0&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&\bar1&0\\1&0&0\\0&0&1\end{pmatrix}$

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).

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

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

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 A1.4.2.5. *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**	$\begin{pmatrix}\bar1&0&0\\0&0&\bar1\\0&\bar1&0\end{pmatrix}$
	2″	**b** + **c**	$\begin{pmatrix}\bar1&0&0\\0&0&1\\0&1&0\end{pmatrix}$
N^y	*2*′	**a** − **c**	$\begin{pmatrix}0&0&\bar1\\0&\bar1&0\\\bar1&0&0\end{pmatrix}$
	2″	**a** + **c**	$\begin{pmatrix}0&0&1\\0&\bar1&0\\1&0&0\end{pmatrix}$
N^z	*2*′	**a** − **b**	$\begin{pmatrix}0&\bar1&0\\\bar1&0&0\\0&0&\bar1\end{pmatrix}$
	2″	**a** + **b**	$\begin{pmatrix}0&1&0\\1&0&0\\0&0&\bar1\end{pmatrix}$

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

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