The formulae for the combination of affine mappings and for the inverse of an affine mapping (regular matrix $\boldsymbol{W}$) are obtained by

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}_1\,\boldsymbol{x} + \boldsymbol{w}_1,\ \tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{W}_2\,\tilde{\boldsymbol{x}} + \boldsymbol{w}_2 = \boldsymbol{W}_3\,\boldsymbol{x} + \boldsymbol{w}_3$$
$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{W}_2\,(\boldsymbol{W}_1\,\boldsymbol{x} + \boldsymbol{w}_1) + \boldsymbol{w}_2 = \boldsymbol{W}_2\,\boldsymbol{W}_1\,\boldsymbol{x} + \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2.$$

From $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, it follows that $\boldsymbol{W}^{-1}\,\tilde{\boldsymbol{x}} = \boldsymbol{x} + \boldsymbol{W}^{-1}\,\boldsymbol{w}$ or $\boldsymbol{x} = \boldsymbol{W}^{-1}\,\tilde{\boldsymbol{x}} - \boldsymbol{W}^{-1}\,\boldsymbol{w}$.

Using matrix–column pairs, this reads

$$(\boldsymbol{W}_3,\,\boldsymbol{w}_3) = (\boldsymbol{W}_2,\,\boldsymbol{w}_2)\,(\boldsymbol{W}_1,\,\boldsymbol{w}_1) = (\boldsymbol{W}_2\boldsymbol{W}_1,\ \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2) \qquad (1.2.2.5)$$

and

$$\boldsymbol{x} = (\boldsymbol{W},\,\boldsymbol{w})^{-1}\tilde{\boldsymbol{x}} = (\boldsymbol{W}',\,\boldsymbol{w}')\tilde{x}$$

or

$$(\boldsymbol{W}',\,\boldsymbol{w}') = (\boldsymbol{W},\,\boldsymbol{w})^{-1} = (\boldsymbol{W}^{-1},\ -\boldsymbol{W}^{-1}\boldsymbol{w}). \qquad (1.2.2.6)$$

One finds from equations (1.2.2.5) and (1.2.2.6) that the linear parts of the matrix–column pairs transform as one would expect:

(1) the linear part of the product of two matrix–column pairs is the product of the linear parts, *i.e.* if $(\boldsymbol{W}_3,\,\boldsymbol{w}_3) = (\boldsymbol{W}_2,\,\boldsymbol{w}_2)\,(\boldsymbol{W}_1,\,\boldsymbol{w}_1)$ then $\boldsymbol{W}_3 = \boldsymbol{W}_2\,\boldsymbol{W}_1$;

(2) the linear part of the inverse of a matrix–column pair is the inverse of the linear part, *i.e.* if $(\boldsymbol{X},\,\boldsymbol{x}) = (\boldsymbol{W},\,\boldsymbol{w})^{-1}$, then $\boldsymbol{X} = \boldsymbol{W}^{-1}$. [This relation is included in the first one: from $(\boldsymbol{W},\,\boldsymbol{w})\,(\boldsymbol{X},\,\boldsymbol{x}) = (\boldsymbol{W}\boldsymbol{X}, \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}) = (\boldsymbol{I},\,\boldsymbol{o})$ follows $\boldsymbol{X} = \boldsymbol{W}^{-1}$. Here $\boldsymbol{I}$ is the unit matrix and $\boldsymbol{o}$ is the column consisting of zeroes].

These relations will be used in Section 1.2.5.4.

For the column parts, equations (1.2.2.5) and (1.2.2.6) are less convenient:

$$(1)\ \boldsymbol{w}_3 = \boldsymbol{W}_2\,\boldsymbol{w}_1 + \boldsymbol{w}_2; \qquad (2)\ \boldsymbol{w}' = -\boldsymbol{W}^{-1}\boldsymbol{w}.$$

Because of the inconvenience of these relations, it is often preferable to use 'augmented' matrices, by which one can describe the combination of affine mappings and the inverse mapping by the equations of the usual matrix multiplication. These matrices are introduced in the next section.

1.2.2.4. *Matrix–column pairs and $(n+1)\times(n+1)$ matrices*

It is natural to combine the matrix part and the column part describing an affine mapping to form a (3×4) matrix, but such matrices cannot be multiplied by the usual matrix multiplication and cannot be inverted. However, if one supplements the (3×4) matrix by a fourth row '0 0 0 1', one obtains a (4×4) square matrix which can be combined with the analogous matrices of other mappings and can be inverted. These matrices are called *augmented matrices* and are designated by open-face letters in this volume:

$$\mathbb{W} = \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right),\ \tilde{\mathbb{x}} = \left(\begin{array}{c} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{array}\right),\ \mathbb{x} = \left(\begin{array}{c} x \\ y \\ z \\ \hline 1 \end{array}\right). \qquad (1.2.2.7)$$

In order to write equation (1.2.2.3) as $\tilde{\mathbb{x}} = \mathbb{W}\mathbb{x}$ with the augmented matrices $\mathbb{W}$, the columns $\tilde{\boldsymbol{x}}$ and $\boldsymbol{x}$ also have to be extended to the augmented columns $\mathbb{x}$ and $\tilde{\mathbb{x}}$. Equations (1.2.2.5) and (1.2.2.6) then become

$$\mathbb{W}_3 = \mathbb{W}_2\,\mathbb{W}_1 \ \text{ and } \ (\mathbb{W})^{-1} = (\mathbb{W}^{-1}). \qquad (1.2.2.8)$$

The vertical and horizontal lines in the matrix have no mathematical meaning. They are simply a convenience for separating the matrix part from the column part and from the row '0 0 0 1', and could be omitted.

Augmented matrices are very useful when writing down general formulae which then become more transparent and more elegant. However, the matrix–column pair formalism is, in general, advantageous for practical calculations.

For the augmented columns of vector coefficients, see Section 1.2.2.6.

1.2.2.5. *Isometries*

Isometries are special affine mappings, as in Definition 1.2.2.1.1. The matrix $\boldsymbol{W}$ of an isometry has to fulfil conditions which depend on the coordinate basis. These conditions are:

(1) A basis $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ is characterized by the scalar products $(\mathbf{a}_j\,\mathbf{a}_k)$ of its basis vectors or by its *lattice parameters* $a,\,b,\,c,\,\alpha,\,\beta$ and γ. Here $a,\,b,\,c$ are the lengths of the basis vectors $\mathbf{a}_1,\,\mathbf{a}_2,\,\mathbf{a}_3$ and $\alpha,\,\beta$ and γ are the angles between $\mathbf{a}_2$ and $\mathbf{a}_3$, $\mathbf{a}_3$ and $\mathbf{a}_1$, $\mathbf{a}_1$ and $\mathbf{a}_2$, respectively. The *metric matrix* $\boldsymbol{M}$ (called $\mathbf{G}$ in *IT* A, Chapter 9.1) is the (3×3) matrix which consists of the scalar products of the basis vectors:

$$\boldsymbol{M} = \begin{pmatrix} a^2 & a\,b\,\cos\gamma & a\,c\,\cos\beta \\ b\,a\,\cos\gamma & b^2 & b\,c\,\cos\alpha \\ c\,a\,\cos\beta & c\,b\,\cos\alpha & c^2 \end{pmatrix}.$$

If $\boldsymbol{W}$ is the matrix part of an isometry, referred to the basis $(\mathbf{a}_1,\ \mathbf{a}_2,\ \mathbf{a}_3)$, then $\boldsymbol{W}$ must fulfil the condition $\boldsymbol{W}^{\mathrm{T}}\boldsymbol{M}\,\boldsymbol{W} = \boldsymbol{M}$, where $\boldsymbol{W}^{\mathrm{T}}$ is the transpose of $\boldsymbol{W}$.

(2) For the *determinant* of $\boldsymbol{W}$, $\det(\boldsymbol{W}) = \pm1$ must hold; $\det(\boldsymbol{W}) = +1$ for the identity, translations, rotations and screw rotations; $\det(\boldsymbol{W}) = -1$ for inversions, reflections, glide reflections and rotoinversions.

(3) For the *trace*, $\mathrm{tr}(\boldsymbol{W}) = W_{11} + W_{22} + W_{33} = \pm(1 + 2\cos\varphi)$ holds, where φ is the rotation angle; the $+$ sign applies if $\det(\boldsymbol{W}) = +1$ and the $-$ sign if $\det(\boldsymbol{W}) = -1$.

Algorithms for the determination of the kind of isometry from a given matrix–column pair and for the determination of the matrix–column pair for a given isometry can be found in *IT* A, Part 11 or in Hahn & Wondratschek (1994).

1.2.2.6. *Vectors and vector coefficients*

In crystallography, vectors and their coefficients as well as points and their coordinates are used for the description of crystal structures. Vectors represent translation shifts, distance and Patterson vectors, reciprocal-lattice vectors *etc.* With respect to a given basis a vector has three coefficients. In contrast to the coordinates of a point, these coefficients do not change if the origin of the coordinate system is shifted. In the usual description by columns, the vector coefficients cannot be distinguished from the point coordinates, but in the augmented-column description the difference becomes visible: the vector from the point P to the point Q has the coefficients $v_1 = q_1 - p_1,\ v_2 = q_2 - p_2,\ v_3 = q_3 - p_3,\ 1 - 1$. Thus, the column of the coefficients of a vector is not augmented by '1' but by '0'. Therefore, when the point P is mapped onto the point $\tilde{P}$ by $\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$ according to equation (1.2.2.3), then the vector $\mathbf{v} = \overrightarrow{PQ}$ is mapped onto the vector $\tilde{\mathbf{v}} = \overrightarrow{\tilde{P}\tilde{Q}}$ by transforming its coefficients by $\tilde{\boldsymbol{v}} = \boldsymbol{W}\boldsymbol{v}$, because the coefficients w_j are multiplied by the number '0' augmenting the column $\boldsymbol{v} = (v_j)$. Indeed, the

references