Table 3.5.2.3 (continued)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
15	$B112/n$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			4·1·1
		$\gamma=90^\circ$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, \bar{y}, z$	4·1·2
		$\cos\gamma=-b/a,\ 90^\circ<\gamma<135^\circ$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, 2x-y, z$	4·1·2
		$2\cos\gamma=-a/b,\ 90^\circ<\gamma<135^\circ$	$Cccm$ $(n\,n2/m)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}+y+\frac{1}{4}, y, z+\frac{1}{4}$	4·1·2
		$a=b\sqrt{2},\ \gamma=135^\circ$	$P4_2/mmc$ $(2/m2/m\,n)$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, 2x-y, z;$ $\bar{x}+y+\frac{1}{4}, y, z+\frac{1}{4}$	4·1·4
15	$I112/b$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			4·1·1
		$a<b,\ \gamma=90^\circ$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z$	4·1·2
		$\cos\gamma=-a/b,\ 90^\circ<\gamma<180^\circ$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}+2y, y, z$	4·1·2
		$a=b,\ 90^\circ<\gamma<180^\circ$	$Cccm$ $(n\,n2/m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	4·1·2
		$a=b,\ \gamma=90^\circ$	$P4_2/mmc$ $(2/m2/m\,n)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z;\ y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	4·1·4

For each of the other 38 types of orthorhombic space group (3 types of rectangular plane groups), the type of the affine normalizer corresponds to the type of the highest-symmetry Euclidean normalizers belonging to that space (plane)-group type. Therefore, it may also be symbolized by (possibly modified) Hermann–Mauguin symbols [examples: $\mathcal{N}_{\mathcal{A}}(Pbca) = Pm\overline{3}$, $\mathcal{N}_{\mathcal{A}}(Pccn) = P4/mmm$, $\mathcal{N}_{\mathcal{A}}(Pcc2) = P^14/mmm$].

As the affine normalizer of a monoclinic or triclinic space group (oblique plane group) is not isomorphic to any group of motions, it cannot be characterized by a modified Hermann–Mauguin symbol. It may be described, however, by one or two matrix–column pairs together with the appropriate restrictions on the coefficients. Similar information has been given by Billiet *et al.* (1982) for the standard description of each group. The problem has been discussed in more detail by Gubler (1982*a*,*b*).

In Table 3.5.2.6, the affine normalizers of all triclinic and monoclinic space groups are given. The first two columns correspond to those of Tables 3.5.2.3, 3.5.2.4 or 3.5.2.5. The affine normalizers are completely described in column 3 of Table 3.5.2.6 by one or two general matrix–column pairs. All unimodular matrices and columns used in Table 3.5.2.6 are listed explicitly in Table 3.5.2.7. The matrix–column representation of an affine normalizer consists of all combinations of matrices and columns that originate from the specified pair(s) and from the restrictions on the coefficients. This set of matrix–column pairs has of course to include the symmetry operations of $\mathcal{G}$ as well as of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

The relatively complicated group structure of these affine normalizers has to do with the fact that for the corresponding space groups the permissible basis transformations are more complicated than for space groups of higher crystal systems.

In contrast to orthorhombic space groups, the metric of a triclinic or monoclinic space group cannot be specialized in such a way that all elements of the affine normalizer simultaneously become isometries.

The affine normalizers of the oblique plane groups $p1$ and $p2$ can be described analogously. The corresponding unimodular matrix

$$\begin{pmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{pmatrix}$$

has to be combined with the column

$$\begin{pmatrix} r \\ s \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \end{pmatrix}$$

for the representation of $\mathcal{N}_{\mathcal{A}}(p1)$ and $\mathcal{N}_{\mathcal{A}}(p2)$, respectively. n stands for an integer number, r and s stand for real numbers.

3.5.3. Examples of the use of normalizers

BY E. KOCH AND W. FISCHER

3.5.3.1. Introduction

The Euclidean and the affine normalizer of a space group form the appropriate tool to define equivalence relationships on sets of objects that are not symmetry-equivalent in this space group but 'play the same role' with respect to this group. Two such objects referring to the same space group will be called Euclidean- or affine-equivalent if there exists a Euclidean or affine mapping that maps the two objects onto one another and, in addition, maps the space group onto itself.

3.5.3.2. Equivalent point configurations, equivalent Wyckoff positions and equivalent descriptions of crystal structures

In the crystal structure of copper, all atoms are symmetry-equivalent with respect to space group $Fm\overline{3}m$. The pattern of Cu atoms may be described equally well by Wyckoff position $4a$ 0, 0, 0 or $4b$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. The Euclidean normalizer of $Fm\overline{3}m$ gives the relation between the two descriptions.

Two *point configurations* (crystallographic orbits)[3] of a space group $\mathcal{G}$ are called *Euclidean-* or *$\mathcal{N}_{\mathcal{E}}$-equivalent* (*affine-* or *$\mathcal{N}_{\mathcal{A}}$-equivalent*) if they are mapped onto each other by the Euclidean (affine) normalizer of $\mathcal{G}$.

Affine-equivalent point configurations play the same role with respect to the space-group symmetry, *i.e.* their points are embedded in the pattern of symmetry elements in the same way. Euclidean-equivalent point configurations are congruent and may be interchanged when passing from one description of a crystal structure to another.

[3] For the use of the terms 'point configuration' and 'crystallographic orbit' and a comparison of them, see Koch & Fischer (1985) and Sections 3.4.1 and 3.4.2.