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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
		$\gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, \bar{y}, z$	4·1·2
		$\cos\gamma = -b/a,\ 90° < \gamma < 135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, 2x-y, z$	4·1·2
		$2\cos\gamma = -a/b,\ 90° < \gamma < 135°$	$Cccm$ $(n\,n2/m)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}+y+\frac{1}{4}, y, z+\frac{1}{4}$	4·1·2
		$a = b\sqrt{2},\ \gamma = 135°$	$P4_2/mmc$ $(2/m2/m\,n)$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, 2x-y, z;$ $\bar{x}+y+\frac{1}{4}, y, z+\frac{1}{4}$	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
		$a < b,\ \gamma = 90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z$	4·1·2
		$\cos\gamma = -a/b,\ 90° < \gamma < 180°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}+2y, y, z$	4·1·2
		$a = b,\ 90° < \gamma < 180°$	$Cccm$ $(n\,n2/m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	4·1·2
		$a = b,\ \gamma = 90°$	$P4_2/mmc$ $(2/m2/m\,n)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z;\ y+\frac{1}{4}, x+\frac{1}{4},$ $z+\frac{1}{4}$	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: $\mathcal{N}_{\mathcal{A}}(Pbca) = Pm\bar{3}$, $\mathcal{N}_{\mathcal{A}}(Pccn) = P4/mmm$, $\mathcal{N}_{\mathcal{A}}(Pcc2) = P^14/mmm$].

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 $Fm\bar{3}m$. 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 $Fm\bar{3}m$ 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.

Table 3.5.2.4
Euclidean and chirality-preserving Euclidean normalizers of the orthorhombic space groups

The symbols in parentheses following a space-group symbol refer to the location of the origin ('origin choice' in Chapter 2.3).

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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
16	$P222$	$a \neq b \neq c \neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0		$8 \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/		$8 \cdot 1$
		$a = b \neq c$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0	y, x, z	$8 \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/	$y, x, \bar{z}$	$8 \cdot 2$
		$a = b = c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0	$z, x, y;\ y, x, z$	$8 \cdot 2 \cdot 6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P432$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/	$z, x, y;\ y, x, \bar{z}$	$8 \cdot 6$
17	$P222_1$	$a \neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0		$8 \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/		$8 \cdot 1$
		$a = b$	$P4_2/mmc$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0	$y, x, z + \frac{1}{4}$	$8 \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/	$y, x, \bar{z} + \frac{1}{4}$	$8 \cdot 2$
18	$P2_12_12$	$a \neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0		$8 \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/		$8 \cdot 1$
		$a = b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0	y, x, z	$8 \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/	$y, x, \bar{z}$	$8 \cdot 2$
19	$P2_12_12_1$	$a \neq b \neq c \neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0		$8 \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/		$8 \cdot 1$
		$a = b \neq c$	$P4_2/mmc$ $(2/m\,2/m\,n)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0	$y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$	$8 \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_222$ (222_1)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/	$\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	$8 \cdot 2$
		$a = b = c$	$Pm\bar{3}n$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0	$z, x, y;\ y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$	$8 \cdot 2 \cdot 6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_232$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/	$z, x, y;\ \bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	$8 \cdot 6$
20	$C222_1$	$a \neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0		$4 \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$	/		$4 \cdot 1$
		$a = b$	$P4_2/mmc$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0	$y, x, z + \frac{1}{4}$	$4 \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$	/	$y, x, \bar{z} + \frac{1}{4}$	$4 \cdot 2$
21	$C222$	$a \neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0		$4 \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$	/		$4 \cdot 1$
		$a = b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0	y, x, z	$4 \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$	/	$y, x, \bar{z}$	$4 \cdot 2$
22	$F222$	$a \neq b \neq c \neq a$	$Immm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	0, 0, 0		$4 \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	/		$4 \cdot 1$
		$a = b \neq c$	$I4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	0, 0, 0	y, x, z	$4 \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I422$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	/	$y, x, \bar{z}$	$4 \cdot 2$
		$a = b = c$	$Im\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	0, 0, 0	$z, x, y;\ y, x, z$	$4 \cdot 2 \cdot 6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	/	$z, x, y;\ y, x, \bar{z}$	$4 \cdot 6$
23	$I222$	$a \neq b \neq c \neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$	0, 0, 0		$4 \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$	/		$4 \cdot 1$
		$a = b \neq c$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$	0, 0, 0	y, x, z	$4 \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$	/	$y, x, \bar{z}$	$4 \cdot 2$
		$a = b = c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$	0, 0, 0	$z, x, y;\ y, x, z$	$4 \cdot 2 \cdot 6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P432$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$	/	$z, x, y;\ y, x, \bar{z}$	$4 \cdot 6$
24	$I2_12_12_1$	$a \neq b \neq c \neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$	0, 0, 0		$4 \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$	/		$4 \cdot 1$
		$a = b \neq c$	$P4_2/mmc$ $(2/m\,2/m\,n)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$	0, 0, 0	$y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$	$4 \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_222$ (222_1)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$	/	$\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	$4 \cdot 2$
		$a = b = c$	$Pm\bar{3}n$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$	0, 0, 0	$z, x, y;\ y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$	$4 \cdot 2 \cdot 6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_232$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$	/	$z, x, y;\ \bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	$4 \cdot 6$
25	$Pmm2$	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	0, 0, 0		$(4 \cdot \infty) \cdot 2 \cdot 1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	0, 0, 0	y, x, z	$(4 \cdot \infty) \cdot 2 \cdot 2$
26	$Pmc2_1$		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	0, 0, 0		$(4 \cdot \infty) \cdot 2 \cdot 1$
27	$Pcc2$	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	0, 0, 0		$(4 \cdot \infty) \cdot 2 \cdot 1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	0, 0, 0	y, x, z	$(4 \cdot \infty) \cdot 2 \cdot 2$

Table 3.5.2.4 (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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
28	$Pma2$		P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(4\cdot\infty)\cdot 2\cdot 1$
29	$Pca2_1$		P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(4\cdot\infty)\cdot 2\cdot 1$
30	$Pnc2$		P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(4\cdot\infty)\cdot 2\cdot 1$
31	$Pmn2_1$		P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(4\cdot\infty)\cdot 2\cdot 1$
32	$Pba2$	$a \neq b$	P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(4\cdot\infty)\cdot 2\cdot 1$
		$a = b$	P^14/mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	y, x, z	$(4\cdot\infty)\cdot 2\cdot 2$
33	$Pna2_1$		P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(4\cdot\infty)\cdot 2\cdot 1$
34	$Pnn2$	$a \neq b$	P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(4\cdot\infty)\cdot 2\cdot 1$
		$a = b$	P^14/mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	y, x, z	$(4\cdot\infty)\cdot 2\cdot 2$
35	$Cmm2$	$a \neq b$	P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
		$a = b$	P^14/mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
36	$Cmc2_1$		P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
37	$Ccc2$	$a \neq b$	P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
		$a = b$	P^14/mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
38	$Amm2$		P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
39	$Aem2$		P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
40	$Ama2$		P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
41	$Aea2$		P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
42	$Fmm2$	$a \neq b$	P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty\cdot 2\cdot 1$
		$a = b$	P^14/mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$	y, x, z	$\infty\cdot 2\cdot 2$
43	$Fdd2$	$a \neq b$	P^1ban (222)	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$\tfrac{1}{8}, \tfrac{1}{8}, 0$		$\infty\cdot 2\cdot 1$
		$a = b$	P^14/nbm ($\bar{4}2m$)	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$\tfrac{1}{8}, \tfrac{1}{8}, 0$	y, x, z	$\infty\cdot 2\cdot 2$
44	$Imm2$	$a \neq b$	P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
		$a = b$	P^14/mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
45	$Iba2$	$a \neq b$	P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
		$a = b$	P^14/mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
46	$Ima2$		P^1mmm	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
47	$Pmmm$	$a \neq b \neq c \neq a$	$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
		$a = b \neq c$	$P4/mmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
		$a = b = c$	$Pm\bar{3}m$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$		$z, x, y;\ y, x, z$	$8\cdot 1\cdot 6$
48	$Pnnn$ (both origins)	$a \neq b \neq c \neq a$	$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
		$a = b \neq c$	$P4/mmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
		$a = b = c$	$Pm\bar{3}m$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$		$z, x, y;\ y, x, z$	$8\cdot 1\cdot 6$
49	$Pccm$	$a \neq b$	$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
		$a = b$	$P4/mmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
50	$Pban$ (both origins)	$a \neq b$	$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
		$a = b$	$P4/mmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
51	$Pmma$		$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
52	$Pnna$		$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
53	$Pmna$		$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
54	$Pcca$		$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
55	$Pbam$	$a \neq b$	$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
		$a = b$	$P4/mmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
56	$Pccn$	$a \neq b$	$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
		$a = b$	$P4/mmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
57	$Pbcm$		$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
58	$Pnnm$	$a \neq b$	$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
		$a = b$	$P4/mmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
59	$Pmmn$ (both origins)	$a \neq b$	$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$
		$a = b$	$P4/mmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
60	$Pbcn$		$Pmmm$	$\tfrac{1}{2}\mathbf{a}, \tfrac{1}{2}\mathbf{b}, \tfrac{1}{2}\mathbf{c}$	$\tfrac{1}{2}, 0, 0;\ 0, \tfrac{1}{2}, 0;\ 0, 0, \tfrac{1}{2}$			$8\cdot 1\cdot 1$

Table 3.5.2.4 (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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
61	*Pbca*	$a \neq b$ or $b \neq c$ or $a \neq c$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
		$a = b = c$	$Pm\bar{3}$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		z, x, y	$8 \cdot 1 \cdot 3$
62	*Pnma*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
63	*Cmcm*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
64	*Cmce*		*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
65	*Cmmm*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$		y, x, z	$4 \cdot 1 \cdot 2$
66	*Cccm*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$		y, x, z	$4 \cdot 1 \cdot 2$
67	*Cmme*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm* (*mmm*)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$		$y + \frac{1}{4}, x - \frac{1}{4}, z$	$4 \cdot 1 \cdot 2$
68	*Ccce* (222)	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$		y, x, z	$4 \cdot 1 \cdot 2$
68	*Ccce* ($\bar{1}$)	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm* (*mmm*)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$		$y + \frac{1}{4}, x - \frac{1}{4}, z$	$4 \cdot 1 \cdot 2$
69	*Fmmm*	$a \neq b \neq c \neq a$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$			$2 \cdot 1 \cdot 1$
		$a = b \neq c$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$		y, x, z	$2 \cdot 1 \cdot 2$
		$a = b = c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$		$z, x, y;\ y, x, z$	$2 \cdot 1 \cdot 6$
70	*Fddd* (222)	$a \neq b \neq c \neq a$	*Pnnn* (222)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$			$2 \cdot 1 \cdot 1$
		$a = b \neq c$	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$		$\bar{y}, \bar{x}, z$	$2 \cdot 1 \cdot 2$
		$a = b = c$	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$		$z, x, y;\ y, x, z$	$2 \cdot 1 \cdot 6$
70	*Fddd* ($\bar{1}$)	$a \neq b \neq c \neq a$	*Pnnn* ($\bar{1}$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$			$2 \cdot 1 \cdot 1$
		$a = b \neq c$	$P4_2/nnm$ ($2/m$ at $0, \frac{1}{2}, 0$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$		y, x, z	$2 \cdot 1 \cdot 2$
		$a = b = c$	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$		$z, x, y;\ y, x, z$	$2 \cdot 1 \cdot 6$
71	*Immm*	$a \neq b \neq c \neq a$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			$4 \cdot 1 \cdot 1$
		$a = b \neq c$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		y, x, z	$4 \cdot 1 \cdot 2$
		$a = b = c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$z, x, y;\ y, x, z$	$4 \cdot 1 \cdot 6$
72	*Ibam*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			$4 \cdot 1 \cdot 1$
		$a = b$	*P4/mmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		y, x, z	$4 \cdot 1 \cdot 2$
73	*Ibca*	$a \neq b \neq c \neq a$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			$4 \cdot 1 \cdot 1$
		$a = b \neq c$	$P4_2/mmc$ ($2/m\,2/m\,n$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$	$4 \cdot 1 \cdot 2$
		$a = b = c$	$Pm\bar{3}n$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$z, x, y;\ y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$	$4 \cdot 1 \cdot 6$
74	*Imma*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			$4 \cdot 1 \cdot 1$
		$a = b$	$P4_2/mmc$ ($2/m\,2/m\,n$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$y + \frac{1}{4}, x - \frac{1}{4}, z + \frac{1}{4}$	$4 \cdot 1 \cdot 2$

Starting from any given point configuration of a space group $\mathcal{G}$, one may derive all Euclidean-equivalent point configurations and – except for monoclinic and triclinic space groups – all affine-equivalent ones by successive application of the 'additional generators' of the normalizer as given in Tables 3.5.2.3, 3.5.2.4 and 3.5.2.5.

Examples

(1) A point configuration $F\bar{4}3m$ $16e$ x, x, x with $x_1 = 0.10$ may be visualized as a set of parallel tetrahedra arranged in a cubic face-centred lattice. The Euclidean and affine normalizer of $F\bar{4}3m$ is $Im\bar{3}m$ with $a' = \frac{1}{2}a$ (*cf.* Table 3.5.2.5). Since the index k_g of $\mathcal{G}$ in $\mathcal{K}(\mathcal{G})$ is 4, three additional equivalent point configurations exist, which follow from the original one by repeated application of the tabulated translation $t(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$: $16e$ x, x, x with $x_2 = 0.35$, $x_3 = 0.60$, $x_4 = 0.85$. $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{K}(\mathcal{G})$ and an additional centre of symmetry is located at 0, 0, 0. Accordingly, the following four equivalent point configurations may be derived from the first four: $16e$ x, x, x with $x_5 = -0.10$, $x_6 = -0.35$, $x_7 = -0.60$, $x_8 = -0.85$. In this case, the index 8 of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ equals the number of Euclidean-equivalent point configurations.

(2) $F\bar{4}3m$ $4a$ 0, 0, 0 represents a face-centred cubic lattice. The additional translations of $\mathcal{K}(F\bar{4}3m)$ generate three equivalent point configurations: $4c$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$, $4b$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ and $4d$ $\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$. Inversion through 0, 0, 0 maps $4a$ and $4b$ each onto itself and interchanges $4c$ and $4d$. Therefore, here the number of equivalent point configurations is four, *i.e.* only half the index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

The difference between the two examples is the following: The reference point 0.1, 0.1, 0.1 of the first example does not change its site symmetry $.3m$ when passing from $F\bar{4}3m$ to $Im\bar{3}m$. Point 0, 0, 0 of the second example, however, has site symmetry $\bar{4}3m$ in $F\bar{4}3m$, but $m\bar{3}m$ in $Im\bar{3}m$.

(*continued on page* 846)

Table 3.5.2.5
Euclidean and chirality-preserving Euclidean normalizers of the tetragonal, trigonal, hexagonal and cubic space groups
The symbols in parentheses following a space-group symbol refer to the location of the origin ('origin choice' in Chapter 2.3).

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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
75	$P4$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1422	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	/	$y, x, \bar{z}$	$(2\cdot\infty)\cdot 2$
76	$P4_1$	P^1422 [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	/	$y, x, \bar{z}$	$(2\cdot\infty)\cdot 2$
77	$P4_2$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1422	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	/	$y, x, \bar{z}$	$(2\cdot\infty)\cdot 2$
78	$P4_3$	P^1422 [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	/	$y, x, \bar{z}$	$(2\cdot\infty)\cdot 2$
79	$I4$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$	y, x, z	$\infty\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1422	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, \bar{z}$	$\infty\cdot 2$
80	$I4_1$	P^14/nbm ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$\frac{1}{4}, 0, 0$	$y, x, \bar{z}$	$\infty\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1422 (222)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, \bar{z}$	$\infty\cdot 2$
81	$P\bar{4}$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	y, x, z	$4\cdot 2\cdot 2$
82	$I\bar{4}$	$I4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, \frac{1}{4}$	$0, 0, 0$	y, x, z	$4\cdot 2\cdot 2$
83	$P4/m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		y, x, z	$4\cdot 1\cdot 2$
84	$P4_2/m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		y, x, z	$4\cdot 1\cdot 2$
85	$P4/n$ ($\bar{4}$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		y, x, z	$4\cdot 1\cdot 2$
85	$P4/n$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		y, x, z	$4\cdot 1\cdot 2$
86	$P4_2/n$ ($\bar{4}$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		y, x, z	$4\cdot 1\cdot 2$
86	$P4_2/n$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		y, x, z	$4\cdot 1\cdot 2$
87	$I4/m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		y, x, z	$2\cdot 1\cdot 2$
88	$I4_1/a$ ($\bar{4}$)	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$y, x, \bar{z}$	$2\cdot 1\cdot 2$
88	$I4_1/a$ ($\bar{1}$)	$P4_2/nnm$ ($2/m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$2\cdot 1\cdot 2$
89	$P422$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/		$4\cdot 1$
90	$P42_12$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/		$4\cdot 1$
91	$P4_122$	$P4_222$ (222 at 4_212) [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/		$4\cdot 1$
92	$P4_12_12$	$P4_222$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/		$4\cdot 1$
93	$P4_222$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/		$4\cdot 1$
94	$P4_22_12$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/		$4\cdot 1$
95	$P4_322$	$P4_222$ (222 at 4_212) [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/		$4\cdot 1$
96	$P4_32_12$	$P4_222$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	/		$4\cdot 1$
97	$I422$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$0, 0, 0$		$2\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2\cdot 1$
98	$I4_122$	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$\frac{1}{4}, 0, \frac{1}{8}$		$2\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_222$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2\cdot 1$
99	$P4mm$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
100	$P4bm$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
101	$P4_2cm$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
102	$P4_2nm$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
103	$P4cc$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
104	$P4nc$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
105	$P4_2mc$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
106	$P4_2bc$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
107	$I4mm$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty\cdot 2\cdot 1$
108	$I4cm$	P^14/mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty\cdot 2\cdot 1$
109	$I4_1md$	P^14/nbm ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$\frac{1}{4}, 0, 0$		$\infty\cdot 2\cdot 1$
110	$I4_1cd$	P^14/nbm ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$\frac{1}{4}, 0, 0$		$\infty\cdot 2\cdot 1$
111	$P\bar{4}2m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
112	$P\bar{4}2c$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$
113	$P\bar{4}2_1m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$		$4\cdot 2\cdot 1$

Table 3.5.2.5 (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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
114	$P\bar{4}2_1c$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot 2\cdot 1$
115	$P\bar{4}m2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot 2\cdot 1$
116	$P\bar{4}c2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot 2\cdot 1$
117	$P\bar{4}b2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot 2\cdot 1$
118	$P\bar{4}n2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot 2\cdot 1$
119	$I\bar{4}m2$	$I4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,\frac{1}{4}$	$0,0,0$		$4\cdot 2\cdot 1$
120	$I\bar{4}c2$	$I4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,\frac{1}{4}$	$0,0,0$		$4\cdot 2\cdot 1$
121	$I\bar{4}2m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	$0,0,0$		$2\cdot 2\cdot 1$
122	$I\bar{4}2d$	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	$\frac{1}{4},0,\frac{1}{8}$		$2\cdot 2\cdot 1$
123	$P4/mmm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
124	$P4/mcc$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
125	$P4/nbm$ (422)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
125	$P4/nbm$ ($2/m$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
126	$P4/nnc$ (422)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
126	$P4/nnc$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
127	$P4/mbm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
128	$P4/mnc$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
129	$P4/nmm$ ($\bar{4}m2$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
129	$P4/nmm$ ($2/m$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
130	$P4/ncc$ ($\bar{4}$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
130	$P4/ncc$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
131	$P4_2/mmc$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
132	$P4_2/mcm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
133	$P4_2/nbc$ ($\bar{4}$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
133	$P4_2/nbc$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
134	$P4_2/nnm$ ($\bar{4}2m$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
134	$P4_2/nnm$ ($2/m$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
135	$P4_2/mbc$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
136	$P4_2/mnm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
137	$P4_2/nmc$ ($\bar{4}m2$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
137	$P4_2/nmc$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
138	$P4_2/ncm$ ($\bar{4}$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
138	$P4_2/ncm$ ($2/m$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot 1\cdot 1$
139	$I4/mmm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot 1\cdot 1$
140	$I4/mcm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot 1\cdot 1$
141	$I4_1/amd$ ($\bar{4}m2$)	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot 1\cdot 1$
141	$I4_1/amd$ ($2/m$)	$P4_2/nnm$ ($2/m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot 1\cdot 1$
142	$I4_1/acd$ ($\bar{4}$)	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot 1\cdot 1$
142	$I4_1/acd$ ($\bar{1}$)	$P4_2/nnm$ ($2/m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot 1\cdot 1$
143	$P3$	P^16/mmm	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \varepsilon\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0;\ 0,0,t$	$0,0,0$	$\bar{x},\bar{y},z;\ y,x,z$	$(3\cdot\infty)\cdot 2\cdot 4$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1622	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \varepsilon\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0;\ 0,0,t$	/	$\bar{x},\bar{y},z;\ y,x,\bar{z}$	$(3\cdot\infty)\cdot 4$
144	$P3_1$	P^1622 [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \varepsilon\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0;\ 0,0,t$	/	$\bar{x},\bar{y},z;\ y,x,\bar{z}$	$(3\cdot\infty)\cdot 4$
145	$P3_2$	P^1622 [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \varepsilon\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0;\ 0,0,t$	/	$\bar{x},\bar{y},z;\ y,x,\bar{z}$	$(3\cdot\infty)\cdot 4$
146	$R3$ (hexag.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$	$\bar{y},\bar{x},z$	$\infty\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1312	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \varepsilon\mathbf{c}$	$0,0,t$	/	$y,x,\bar{z}$	$\infty\cdot 2$
146	$R3$ (rhomboh.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}-\frac{1}{3}\mathbf{b}-\frac{1}{3}\mathbf{c},\ -\frac{1}{3}\mathbf{a}+\frac{2}{3}\mathbf{b}-\frac{1}{3}\mathbf{c},\ \varepsilon(\mathbf{a}+\mathbf{b}+\mathbf{c})$	r,r,r	$0,0,0$	y,x,z	$\infty\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1312	$\frac{2}{3}\mathbf{a}-\frac{1}{3}\mathbf{b}-\frac{1}{3}\mathbf{c},\ -\frac{1}{3}\mathbf{a}+\frac{2}{3}\mathbf{b}-\frac{1}{3}\mathbf{c},\ \varepsilon(\mathbf{a}+\mathbf{b}+\mathbf{c})$	r,r,r	/	$\bar{y},\bar{x},\bar{z}$	$\infty\cdot 2$
147	$P\bar{3}$	$P6/mmm$	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		$\bar{x},\bar{y},z;\ y,x,z$	$2\cdot 1\cdot 4$
148	$R\bar{3}$ (hexag.)	$R\bar{3}m$ (hexag.)	$-\mathbf{a},\ -\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		$\bar{y},\bar{x},z$	$2\cdot 1\cdot 2$
148	$R\bar{3}$ (rhomboh.)	$R\bar{3}m$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),\ \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		y,x,z	$2\cdot 1\cdot 2$

Table 3.5.2.5 (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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
149	*P*312	*P*6/*mmm*	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0	$\bar{x}, \bar{y}, z$	$6 \cdot 2 \cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: *P*622	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0;\ 0, 0, \frac{1}{2}$	/	$\bar{x}, \bar{y}, z$	$6 \cdot 2$
150	*P*321	*P*6/*mmm*	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	0, 0, 0	$\bar{x}, \bar{y}, z$	$2 \cdot 2 \cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: *P*622	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/	$\bar{x}, \bar{y}, z$	$2 \cdot 2$
151	$P3_112$	$P6_222$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0;\ 0, 0, \frac{1}{2}$	/	$\bar{x}, \bar{y}, z$	$6 \cdot 2$
152	$P3_121$	$P6_222$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}+\mathbf{b},\ -\mathbf{a},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/	$\bar{x}, \bar{y}, z$	$2 \cdot 2$
153	$P3_212$	$P6_422$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0;\ 0, 0, \frac{1}{2}$	/	$\bar{x}, \bar{y}, z$	$6 \cdot 2$
154	$P3_221$	$P6_422$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}+\mathbf{b},\ -\mathbf{a},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/	$\bar{x}, \bar{y}, z$	$2 \cdot 2$
155	*R*32 (hexag.)	$R\bar{3}m$ (hexag.)	$-\mathbf{a},\ -\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	0, 0, 0		$2 \cdot 2 \cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: *R*32 (hexag.)	$-\mathbf{a},\ -\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2 \cdot 1$
155	*R*32 (rhomboh.)	$R\bar{3}m$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),\ \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0		$2 \cdot 2 \cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: *R*32 (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),\ \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/		$2 \cdot 1$
156	*P*3*m*1	P^16/mmm	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \varepsilon\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}, \bar{y}, z$	$(3 \cdot \infty) \cdot 2 \cdot 2$
157	*P*31*m*	P^16/mmm	$\mathbf{a},\ \mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	0, 0, 0	$\bar{x}, \bar{y}, z$	$\infty \cdot 2 \cdot 2$
158	*P*3*c*1	P^16/mmm	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \varepsilon\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}, \bar{y}, z$	$(3 \cdot \infty) \cdot 2 \cdot 2$
159	*P*31*c*	P^16/mmm	$\mathbf{a},\ \mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	0, 0, 0	$\bar{x}, \bar{y}, z$	$\infty \cdot 2 \cdot 2$
160	*R*3*m* (hexag.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	0, 0, 0		$\infty \cdot 2 \cdot 1$
160	*R*3*m* (rhomboh.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}-\frac{1}{3}\mathbf{b}-\frac{1}{3}\mathbf{c},\ -\frac{1}{3}\mathbf{a}+\frac{2}{3}\mathbf{b}-\frac{1}{3}\mathbf{c},\ \varepsilon(\mathbf{a}+\mathbf{b}+\mathbf{c})$	r, r, r	0, 0, 0		$\infty \cdot 2 \cdot 1$
161	*R*3*c* (hexag.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	0, 0, 0		$\infty \cdot 2 \cdot 1$
161	*R*3*c* (rhomboh.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}-\frac{1}{3}\mathbf{b}-\frac{1}{3}\mathbf{c},\ -\frac{1}{3}\mathbf{a}+\frac{2}{3}\mathbf{b}-\frac{1}{3}\mathbf{c},\ \varepsilon(\mathbf{a}+\mathbf{b}+\mathbf{c})$	r, r, r	0, 0, 0		$\infty \cdot 2 \cdot 1$
162	$P\bar{3}1m$	*P*6/*mmm*	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$\bar{x}, \bar{y}, z$	$2 \cdot 1 \cdot 2$
163	$P\bar{3}1c$	*P*6/*mmm*	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$\bar{x}, \bar{y}, z$	$2 \cdot 1 \cdot 2$
164	$P\bar{3}m1$	*P*6/*mmm*	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$\bar{x}, \bar{y}, z$	$2 \cdot 1 \cdot 2$
165	$P\bar{3}c1$	*P*6/*mmm*	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$\bar{x}, \bar{y}, z$	$2 \cdot 1 \cdot 2$
166	$R\bar{3}m$ (hexag.)	$R\bar{3}m$ (hexag.)	$-\mathbf{a},\ -\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
166	$R\bar{3}m$ (rhomboh.)	$R\bar{3}m$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),\ \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
167	$R\bar{3}c$ (hexag.)	$R\bar{3}m$ (hexag.)	$-\mathbf{a},\ -\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
167	$R\bar{3}c$ (rhomboh.)	$R\bar{3}m$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c}),\ \frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
168	*P*6	P^16/mmm	$\mathbf{a},\ \mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	0, 0, 0	y, x, z	$\infty \cdot 2 \cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1622	$\mathbf{a},\ \mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, \bar{z}$	$\infty \cdot 2$
169	$P6_1$	P^1622 [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a},\ \mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, \bar{z}$	$\infty \cdot 2$
170	$P6_5$	P^1622 [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a},\ \mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, \bar{z}$	$\infty \cdot 2$
171	$P6_2$	P^1622 [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a},\ \mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, \bar{z}$	$\infty \cdot 2$
172	$P6_4$	P^1622 [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a},\ \mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, \bar{z}$	$\infty \cdot 2$
173	$P6_3$	P^16/mmm	$\mathbf{a},\ \mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	0, 0, 0	y, x, z	$\infty \cdot 2 \cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1622	$\mathbf{a},\ \mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	/	$y, x, \bar{z}$	$\infty \cdot 2$
174	$P\bar{6}$	*P*6/*mmm*	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0	y, x, z	$6 \cdot 2 \cdot 2$
175	*P*6/*m*	*P*6/*mmm*	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
176	$P6_3/m$	*P*6/*mmm*	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
177	*P*622	*P*6/*mmm*	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	0, 0, 0		$2 \cdot 2 \cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: *P*622	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2 \cdot 1$
178	$P6_122$	$P6_222$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2 \cdot 1$
179	$P6_522$	$P6_422$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2 \cdot 1$
180	$P6_222$	$P6_422$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2 \cdot 1$
181	$P6_422$	$P6_222$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2 \cdot 1$
182	$P6_322$	*P*6/*mmm*	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	0, 0, 0		$2 \cdot 2 \cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: *P*622	$\mathbf{a},\ \mathbf{b},\ \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2 \cdot 1$
183	*P*6*mm*	P^16/mmm	$\mathbf{a},\ \mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	0, 0, 0		$\infty \cdot 2 \cdot 1$
184	*P*6*cc*	P^16/mmm	$\mathbf{a},\ \mathbf{b},\ \varepsilon\mathbf{c}$	$0, 0, t$	0, 0, 0		$\infty \cdot 2 \cdot 1$

Table 3.5.2.5 (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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
185	$P6_3cm$	P^16/mmm	**a**, **b**, ε**c**	$0, 0, t$	0, 0, 0		$\infty \cdot 2 \cdot 1$
186	$P6_3mc$	P^16/mmm	**a**, **b**, ε**c**	$0, 0, t$	0, 0, 0		$\infty \cdot 2 \cdot 1$
187	$P\bar{6}m2$	$P6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0		$6 \cdot 2 \cdot 1$
188	$P\bar{6}c2$	$P6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0;\ 0, 0, \frac{1}{2}$	0, 0, 0		$6 \cdot 2 \cdot 1$
189	$P\bar{6}2m$	$P6/mmm$	**a**, **b**, $\frac{1}{2}$**c**	$0, 0, \frac{1}{2}$	0, 0, 0		$2 \cdot 2 \cdot 1$
190	$P\bar{6}2c$	$P6/mmm$	**a**, **b**, $\frac{1}{2}$**c**	$0, 0, \frac{1}{2}$	0, 0, 0		$2 \cdot 2 \cdot 1$
191	$P6/mmm$	$P6/mmm$	**a**, **b**, $\frac{1}{2}$**c**	$0, 0, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
192	$P6/mcc$	$P6/mmm$	**a**, **b**, $\frac{1}{2}$**c**	$0, 0, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
193	$P6_3/mcm$	$P6/mmm$	**a**, **b**, $\frac{1}{2}$**c**	$0, 0, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
194	$P6_3/mmc$	$P6/mmm$	**a**, **b**, $\frac{1}{2}$**c**	$0, 0, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
195	$P23$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0	y, x, z	$2 \cdot 2 \cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/	$y, x, \bar{z}$	$2 \cdot 2$
196	$F23$	$Im\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	0, 0, 0	y, x, z	$4 \cdot 2 \cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	/	$y, x, \bar{z}$	$4 \cdot 2$
197	$I23$	$Im\bar{3}m$	**a**, **b**, **c**		0, 0, 0	y, x, z	$1 \cdot 2 \cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	**a**, **b**, **c**		/	$y, x, \bar{z}$	$1 \cdot 2$
198	$P2_13$	$Ia\bar{3}d$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0	$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$2 \cdot 2 \cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I4_132$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/	$\bar{y}+\frac{1}{4}, \bar{x}+\frac{1}{4}, \bar{z}+\frac{1}{4}$	$2 \cdot 2$
199	$I2_13$	$Ia\bar{3}d$	**a**, **b**, **c**		0, 0, 0	$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$1 \cdot 2 \cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I4_132$	**a**, **b**, **c**		/	$\bar{y}+\frac{1}{4}, \bar{x}+\frac{1}{4}, \bar{z}+\frac{1}{4}$	$1 \cdot 2$
200	$Pm\bar{3}$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
201	$Pn\bar{3}$ (23)	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
201	$Pn\bar{3}$ ($\bar{3}$)	$Im\bar{3}m$ ($\bar{3}m$)	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
202	$Fm\bar{3}$	$Pm\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
203	$Fd\bar{3}$ (23)	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
203	$Fd\bar{3}$ ($\bar{3}$)	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
204	$Im\bar{3}$	$Im\bar{3}m$	**a**, **b**, **c**			y, x, z	$1 \cdot 1 \cdot 2$
205	$Pa\bar{3}$	$Ia\bar{3}$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
206	$Ia\bar{3}$	$Ia\bar{3}d$	**a**, **b**, **c**			$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$1 \cdot 1 \cdot 2$
207	$P432$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0		$2 \cdot 2 \cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/		$2 \cdot 1$
208	$P4_232$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0		$2 \cdot 2 \cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/		$2 \cdot 1$
209	$F432$	$Pm\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0		$2 \cdot 2 \cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P432$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/		$2 \cdot 1$
210	$F4_132$	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$		$2 \cdot 2 \cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_232$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/		$2 \cdot 1$
211	$I432$	$Im\bar{3}m$	**a**, **b**, **c**		0, 0, 0		$1 \cdot 2 \cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	**a**, **b**, **c**		/		$1 \cdot 1$
212	$P4_332$	$I4_132$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/		$2 \cdot 1$
213	$P4_132$	$I4_132$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/		$2 \cdot 1$
214	$I4_132$	$Ia\bar{3}d$	**a**, **b**, **c**		0, 0, 0		$1 \cdot 2 \cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I4_132$	**a**, **b**, **c**		/		$1 \cdot 1$
215	$P\bar{4}3m$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0		$2 \cdot 2 \cdot 1$
216	$F\bar{4}3m$	$Im\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	0, 0, 0		$4 \cdot 2 \cdot 1$
217	$I\bar{4}3m$	$Im\bar{3}m$	**a**, **b**, **c**		0, 0, 0		$1 \cdot 2 \cdot 1$
218	$P\bar{4}3n$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	0, 0, 0		$2 \cdot 2 \cdot 1$
219	$F\bar{4}3c$	$Im\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	0, 0, 0		$4 \cdot 2 \cdot 1$
220	$I\bar{4}3d$	$Ia\bar{3}d$	**a**, **b**, **c**		0, 0, 0		$1 \cdot 2 \cdot 1$
221	$Pm\bar{3}m$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
222	$Pn\bar{3}n$ (432)	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
222	$Pn\bar{3}n$ ($\bar{3}$)	$Im\bar{3}m$ ($\bar{3}m$)	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
223	$Pm\bar{3}n$	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$

Table 3.5.2.5 (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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
224	$Pn\bar{3}m$ ($\bar{4}3m$)	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
224	$Pn\bar{3}m$ ($\bar{3}m$)	$Im\bar{3}m$ ($\bar{3}m$)	**a**, **b**, **c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
225	$Fm\bar{3}m$	$Pm\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
226	$Fm\bar{3}c$	$Pm\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
227	$Fd\bar{3}m$ ($\bar{4}3m$)	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
227	$Fd\bar{3}m$ ($\bar{3}m$)	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
228	$Fd\bar{3}c$ (23)	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
228	$Fd\bar{3}c$ ($\bar{3}$)	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
229	$Im\bar{3}m$	$Im\bar{3}m$	**a**, **b**, **c**				$1 \cdot 1 \cdot 1$
230	$Ia\bar{3}d$	$Ia\bar{3}d$	**a**, **b**, **c**				$1 \cdot 1 \cdot 1$

The following rule holds without exception: The number of point configurations equivalent to a given one is equal to the quotient i/i_s, with i being the subgroup index of $\mathcal{G}$ in its Euclidean or affine normalizer and i_s the subgroup index between the corresponding two site-symmetry groups of any point in the original point configuration.

When referring to the Euclidean normalizer, i_s may be higher than 1 only if the eigensymmetry of the point configuration under consideration (*i.e.* the group of all motions that maps the point configuration onto itself, *cf.* Sections 1.4.4.4 and 3.4.1.3) is a proper supergroup of $\mathcal{G}$. If $\mathcal{D}$ designates the intersection group of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ with the eigensymmetry group of the point configuration, the number of Euclidean-equivalent point configurations equals the index of $\mathcal{D}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

Example

The Euclidean and affine normalizer of $P2_13$ is $Ia\bar{3}d$ with index 8. Point configuration $4a\ x, x, x$ with $x_1 = 0$ forms a face-centred cubic lattice with eigensymmetry $Fm\bar{3}m$. The reference point $0, 0, 0$ has site symmetry .3. in $P2_13$ but $.\bar{3}.$ in $Ia\bar{3}d$. The number of equivalent point configurations, therefore, is $i/i_s = 8/2 = 4$. One additional point configuration is generated by the translation $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$: $4a\ x, x, x$ with $x_2 = \frac{1}{2}$, the two others by applying the d-glide reflection $y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$ to the first two point configurations: $4a\ x, x, x$ with $x_3 = \frac{1}{4}$ and $x_4 = \frac{3}{4}$. The intersection group $\mathcal{D}$ of the eigensymmetry $Fm\bar{3}m$ with the normalizer $Ia\bar{3}d$ is $Pa\bar{3}$. Its index 4 in $Ia\bar{3}d$ gives again the number of equivalent point configurations.

The set of equivalent point configurations is always infinite if the normalizer contains continuous translations, but this set may be described by a finite number of subsets due to non-continuous translations.

Example

The Euclidean and affine normalizer of $P6_1$ is P^1622 (**a**, **b**, ε**c**). With the aid of the 'additional generators' given in Table 3.5.2.5, one can calculate two subsets of point configurations that are equivalent to a given general point configuration $6a\ x, y, z$ with $x = x_0$, $y = y_0$, $z = z_0$: $6a\ x, y, z$ with $x_0, y_0, z_0 + t$ and $y_0, x_0, -z_0 + t$. If, however, the coordinates for the original point configuration are specialized, *e.g.* to $x = y = x_1$, $z = z_1$ or to $x = y = 0$, $z = z_2$, only one subset exists, namely $x_1, x_1, z_1 + t$ or $0, 0, z_2 + t$, respectively. The reduction of the number of subsets is a consequence of the enhancement of the site symmetry in the normalizer (.2. or 622, respectively), but the index i_s, as introduced above, does not necessarily give the reduction factor for the number of subsets.

It has to be noticed that for most space groups with a Euclidean normalizer containing continuous translations the index i_s is larger than 1 for *all* point configurations, *i.e.* the number of subsets of equivalent point configurations is necessarily reduced. The general Wyckoff position of such a space group does not belong to a characteristic type of Wyckoff sets (*cf.* Sections 1.4.4 and 3.4.1.3) and the eigensymmetry of all corresponding point configurations is enhanced.

Example

The Euclidean and affine normalizer of $P6$ is P^16/mmm (**a**, **b**, ε**c**). As a consequence of the continuous translations, the site symmetry of any point is at least $m..$ in P^16/mmm. With the aid of the 'additional generators', one calculates four subsets of point configurations that are equivalent to a given general point configuration $6d\ x, y, z$ with $x = x_0$, $y = y_0$, $z = z_0$: $x_0, y_0, z_0 + t$; $-x_0, -y_0, -z_0 + t$; $y_0, x_0, z_0 + t$; $-y_0, -x_0, -z_0 + t$. The first two and the second two subsets coincide, however.

According to the above examples, Euclidean- (affine-) equivalent point configurations may or may not belong to the same Wyckoff position. Consequently, normalizers also define equivalence relations on Wyckoff positions:

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

Euclidean-equivalent Wyckoff positions are important for the description or comparison of crystal structures in terms of atomic coordinates. Affine-equivalent Wyckoff positions result in *Wyckoff sets* (*cf.* Sections 1.4.4 and 3.4.1.2) and form the necessary basis for the *definition of lattice complexes.* All site-symmetry groups corresponding to equivalent Wyckoff positions are conjugate in the respective normalizer.

Table 3.5.2.6
Affine normalizers of the triclinic and monoclinic space groups

Space group $\mathcal{G}$ No.	Hermann–Mauguin symbol	Matrix–column pairs in Table 3.5.2.7
1	$P1$	$\boldsymbol{M}_1, \boldsymbol{v}_1$
2	$P\bar{1}$	$\boldsymbol{M}_1, \boldsymbol{v}_2$
3	$P121$	$\boldsymbol{M}_2, \boldsymbol{v}_3$
3	$P112$	$\boldsymbol{M}_3, \boldsymbol{v}_4$
4	$P12_11$	$\boldsymbol{M}_2, \boldsymbol{v}_3$
4	$P112_1$	$\boldsymbol{M}_3, \boldsymbol{v}_4$
5	$C121$	$\boldsymbol{M}_4, \boldsymbol{v}_3$
5	$A121$	$\boldsymbol{M}_5, \boldsymbol{v}_3$
5	$I121$	$\boldsymbol{M}_6, \boldsymbol{v}_3$; $\boldsymbol{M}_7, \boldsymbol{v}_3$
5	$A112$	$\boldsymbol{M}_8, \boldsymbol{v}_4$
5	$B112$	$\boldsymbol{M}_9, \boldsymbol{v}_4$
5	$I112$	$\boldsymbol{M}_{10}, \boldsymbol{v}_4$; $\boldsymbol{M}_{11}, \boldsymbol{v}_4$
6	$P1m1$	$\boldsymbol{M}_2, \boldsymbol{v}_5$
6	$P11m$	$\boldsymbol{M}_3, \boldsymbol{v}_6$
7	$P1c1$	$\boldsymbol{M}_5, \boldsymbol{v}_5$
7	$P1n1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_7, \boldsymbol{v}_5$
7	$P1a1$	$\boldsymbol{M}_4, \boldsymbol{v}_5$
7	$P11a$	$\boldsymbol{M}_9, \boldsymbol{v}_6$
7	$P11n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{11}, \boldsymbol{v}_6$
7	$P11b$	$\boldsymbol{M}_8, \boldsymbol{v}_6$
8	$C1m1$	$\boldsymbol{M}_4, \boldsymbol{v}_5$
8	$A1m1$	$\boldsymbol{M}_5, \boldsymbol{v}_5$
8	$I1m1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_7, \boldsymbol{v}_5$
8	$A11m$	$\boldsymbol{M}_8, \boldsymbol{v}_6$
8	$B11m$	$\boldsymbol{M}_9, \boldsymbol{v}_6$
8	$I11m$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{11}, \boldsymbol{v}_6$
9	$C1c1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_{12}, \boldsymbol{v}_7$
9	$A1n1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_{13}, \boldsymbol{v}_7$
9	$I1a1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_7, \boldsymbol{v}_7$
9	$A11a$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{14}, \boldsymbol{v}_8$
9	$B11n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{15}, \boldsymbol{v}_8$
9	$I11b$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{11}, \boldsymbol{v}_8$
10	$P12/m1$	$\boldsymbol{M}_2, \boldsymbol{v}_2$
10	$P112/m$	$\boldsymbol{M}_3, \boldsymbol{v}_2$
11	$P12_1/m1$	$\boldsymbol{M}_2, \boldsymbol{v}_2$
11	$P112_1/m$	$\boldsymbol{M}_3, \boldsymbol{v}_2$
12	$C12/m1$	$\boldsymbol{M}_4, \boldsymbol{v}_2$
12	$A12/m1$	$\boldsymbol{M}_5, \boldsymbol{v}_2$
12	$I12/m1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_7, \boldsymbol{v}_2$
12	$A112/m$	$\boldsymbol{M}_8, \boldsymbol{v}_2$
12	$B112/m$	$\boldsymbol{M}_9, \boldsymbol{v}_2$
12	$I112/m$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{11}, \boldsymbol{v}_2$
13	$P12/c1$	$\boldsymbol{M}_5, \boldsymbol{v}_2$
13	$P12/n1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_7, \boldsymbol{v}_2$
13	$P12/a1$	$\boldsymbol{M}_4, \boldsymbol{v}_2$
13	$P112/a$	$\boldsymbol{M}_9, \boldsymbol{v}_2$
13	$P112/n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{11}, \boldsymbol{v}_2$
13	$P112/b$	$\boldsymbol{M}_8, \boldsymbol{v}_2$
14	$P12_1/c1$	$\boldsymbol{M}_5, \boldsymbol{v}_2$
14	$P12_1/n1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_7, \boldsymbol{v}_2$
14	$P12_1/a1$	$\boldsymbol{M}_4, \boldsymbol{v}_2$
14	$P112_1/a$	$\boldsymbol{M}_9, \boldsymbol{v}_2$
14	$P112_1/n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{11}, \boldsymbol{v}_2$
14	$P112_1/b$	$\boldsymbol{M}_8, \boldsymbol{v}_2$
15	$C12/c1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_{12}, \boldsymbol{v}_9$
15	$A12/n1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_{13}, \boldsymbol{v}_{10}$
15	$I12/a1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_7, \boldsymbol{v}_{11}$
15	$A112/a$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{14}, \boldsymbol{v}_{10}$
15	$B112/n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{15}, \boldsymbol{v}_{12}$
15	$I112/b$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{11}, \boldsymbol{v}_{11}$

Table 3.5.2.7
Matrices and columns used in Table 3.5.2.6 for the description of the affine normalizers of monoclinic and triclinic space groups

n, *g* and *u* represent integer, even and odd numbers, respectively, *r*, *s* and *t* real numbers. For all matrices, $\det(\boldsymbol{M}_i) = \pm 1$ must hold.

$$\boldsymbol{M}_1 = \begin{pmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{pmatrix} \quad \boldsymbol{M}_2 = \begin{pmatrix} n_{11} & 0 & n_{13} \\ 0 & \pm 1 & 0 \\ n_{31} & 0 & n_{33} \end{pmatrix} \quad \boldsymbol{M}_3 = \begin{pmatrix} n_{11} & n_{12} & 0 \\ n_{21} & n_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_4 = \begin{pmatrix} u_{11} & 0 & n_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{pmatrix} \quad \boldsymbol{M}_5 = \begin{pmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ n_{31} & 0 & u_{33} \end{pmatrix}$$

$$\boldsymbol{M}_6 = \begin{pmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{pmatrix} \quad \boldsymbol{M}_7 = \begin{pmatrix} g_{11} & 0 & u_{13} \\ 0 & \pm 1 & 0 \\ u_{31} & 0 & g_{33} \end{pmatrix} \quad \boldsymbol{M}_8 = \begin{pmatrix} u_{11} & g_{12} & 0 \\ n_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_9 = \begin{pmatrix} u_{11} & n_{12} & 0 \\ g_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_{10} = \begin{pmatrix} u_{11} & g_{12} & 0 \\ g_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$$

$$\boldsymbol{M}_{11} = \begin{pmatrix} g_{11} & u_{12} & 0 \\ u_{21} & g_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_{12} = \begin{pmatrix} u_{11} & 0 & u_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{pmatrix} \quad \boldsymbol{M}_{13} = \begin{pmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ u_{31} & 0 & u_{33} \end{pmatrix} \quad \boldsymbol{M}_{14} = \begin{pmatrix} u_{11} & g_{12} & 0 \\ u_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_{15} = \begin{pmatrix} u_{11} & u_{12} & 0 \\ g_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$$

$$\boldsymbol{v}_1 = \begin{pmatrix} r \\ s \\ t \end{pmatrix} \quad \boldsymbol{v}_2 = \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \\ \frac{1}{2}n_3 \end{pmatrix} \quad \boldsymbol{v}_3 = \begin{pmatrix} \frac{1}{2}n_1 \\ s \\ \frac{1}{2}n_3 \end{pmatrix} \quad \boldsymbol{v}_4 = \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \\ t \end{pmatrix} \quad \boldsymbol{v}_5 = \begin{pmatrix} r \\ \frac{1}{2}n_2 \\ t \end{pmatrix}$$

$$\boldsymbol{v}_6 = \begin{pmatrix} r \\ s \\ \frac{1}{2}n_3 \end{pmatrix} \quad \boldsymbol{v}_7 = \begin{pmatrix} r \\ \frac{1}{4}u_2 \\ t \end{pmatrix} \quad \boldsymbol{v}_8 = \begin{pmatrix} r \\ s \\ \frac{1}{4}u_3 \end{pmatrix} \quad \boldsymbol{v}_9 = \begin{pmatrix} \frac{1}{4}u_1 \\ \frac{1}{4}u_2 \\ \frac{1}{2}n_3 \end{pmatrix} \quad \boldsymbol{v}_{10} = \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{4}u_2 \\ \frac{1}{4}u_3 \end{pmatrix}$$

$$\boldsymbol{v}_{11} = \begin{pmatrix} \frac{1}{4}u_1 \\ \frac{1}{4}u_2 \\ \frac{1}{4}u_3 \end{pmatrix} \quad \boldsymbol{v}_{12} = \begin{pmatrix} \frac{1}{4}u_1 \\ \frac{1}{2}n_2 \\ \frac{1}{4}u_3 \end{pmatrix}$$

Examples

The Euclidean and affine normalizer of $I\bar{4}m2$ is $I4/mmm$ $(\frac{1}{2}\mathbf{a}-\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$. It maps the point configurations $2a$ $0,0,0$, $2b$ $0,0,\frac{1}{2}$, $2c$ $0,\frac{1}{2},\frac{1}{4}$ and $2d$ $0,\frac{1}{2},\frac{3}{4}$ (body-centred tetragonal lattices) onto each other. Accordingly, Wyckoff positions *a* to *d* are affine-equivalent and together form a Wyckoff set. Analogous point configurations exist in subgroup $P\bar{4}n2$ of $I\bar{4}m2$ (again Wyckoff positions *a* to *d*). The Euclidean and affine normalizer of $P\bar{4}n2$, however, is $P4/mmm$ $(\frac{1}{2}\mathbf{a}-\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$, not containing $t(\frac{1}{2},0,\frac{1}{4})$. Therefore, Wyckoff positions *a* and *b* form one Wyckoff set, *c* and *d* a different one. This is also reflected in the site-symmetry groups $\bar{4}$.. and 2.22.

The existence of Euclidean-equivalent point configurations results in different but *equivalent descriptions of crystal structures* (exception: crystal structures with symmetry $Im\bar{3}m$ or $Ia\bar{3}d$). All such equivalent descriptions are derived by applying the additional generators of the Euclidean normalizer of the space group $\mathcal{G}$ to all point configurations of the original description. Since an adequate description of a crystal structure always displays the full symmetry group of that structure, the number of equivalent descriptions must equal the index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

Example

Ag_3PO_4 crystallizes with symmetry $P\bar{4}3n$ (*cf.* Masse *et al.*, 1976): P at $2a$ $0,0,0$, Ag at $6d$ $\frac{1}{4},0,\frac{1}{2}$ and O at $8e$ x,x,x with $x=0.1486$. $\mathcal{N}_{\mathcal{E}}(P\bar{4}3n)=Im\bar{3}m$ with index 4 gives rise to three additional equivalent descriptions: $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ yields P at $2a$ $0,0,0$, Ag at $6c$ $\frac{1}{4},\frac{1}{2},0$ and O at $8e$ x,x,x with $x=0.1486$; inversion through the origin results in P at $2a$ $0,0,0$, Ag at $6d$ $\frac{1}{4},0,\frac{1}{2}$, O at $8e$ x,x,x with $x=-0.1486$ and in P at $2a$ $0,0,0$, Ag at $6c$ $\frac{1}{4},\frac{1}{2},0$ and O at $8e$ x,x,x with $x=-0.1486$. Although the phosphorus configuration is the same for all descriptions and the silver and oxygen atoms refer to only two configurations each, their combinations result in a total of four different equivalent descriptions of the structure.

If the Euclidean normalizer of a space group contains continuous translations, each crystal structure with that symmetry refers to an infinite set of equivalent descriptions. This set may be subdivided into a finite number of subsets in such a way that the descriptions of each subset vary according to the continuous translations. The number of these subsets is given by the product of the finite factors listed in the last column of Tables 3.5.2.3, 3.5.2.4 and 3.5.2.5.

Example

The tetragonal form of $BaTiO_3$ has been described in space group $P4mm$ (*cf. e.g.* Buttner & Maslen, 1992): Ba at $1a$ $0,0,z$ with $z=0$, Ti at $1b$ $\frac{1}{2},\frac{1}{2},z$ with $z=0.482$, O1 at $1b$ $\frac{1}{2},\frac{1}{2},z$ with $z=0.016$, and O2 at $2c$ $\frac{1}{2},0,z$ with $z=0.515$. $\mathcal{N}_{\mathcal{E}}(P4mm)$ $=P^14/mmm$ $(\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c})$ gives rise to $(2\cdot\infty)\cdot 2\cdot 1$ equivalent descriptions of this structure. The continuous translation with vector $(0,0,t)$ yields a first infinite subset of equivalent descriptions: Ba at $1a$ $0,0,z$ with $z=t$, Ti at $1b$ $\frac{1}{2},\frac{1}{2},z$ with $z=0.482+t$, O1 at $1b$ $\frac{1}{2},\frac{1}{2},z$ with $z=0.016+t$, and O2 at $2c$ $\frac{1}{2},0,z$ with $z=0.515+t$. The translation with vector $(\frac{1}{2},\frac{1}{2},0)$ generates a second infinite subset: Ba at $1b$ $\frac{1}{2},\frac{1}{2},z$ with $z=t$, Ti at $1a$ $0,0,z$ with $z=0.482+t$, O1 at $1a$ $0,0,z$ with $z=0.016+t$, and O2 at $2c$ $\frac{1}{2},0,z$ with $z=0.515+t$. Inversion through the origin causes two further infinite subsets of equivalent coordinate descriptions of $BaTiO_3$: first, Ba at $1a$ $0,0,z$ with $z=t$, Ti at $1b$ $\frac{1}{2},\frac{1}{2},z$ with $z=0.518+t$, O1 at $1b$ $\frac{1}{2},\frac{1}{2},z$ with $z=-0.016+t$, and O2 at $2c$ $\frac{1}{2},0,z$ with $z=0.485+t$; second, Ba at $1b$ $\frac{1}{2},\frac{1}{2},z$ with $z=t$, Ti at $1a$ $0,0,z$ with $z=0.518+t$, O1 at $1a$ $0,0,z$ with $z=-0.016+t$, and O2 at $2c$ $\frac{1}{2},0,z$ with $z=0.485+t$.

For any chiral crystal structure two variants with opposite handedness exist and the corresponding symmetry group $\mathcal{G}$ is a Sohncke space group, *i.e.* a group without improper motions. Two cases should be distinguished:

(1) $\mathcal{G}$ is an achiral space group. Then its Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ contains improper motions and interchanges the coordinate descriptions of crystals with different handedness. To obtain equivalent descriptions of the chiral crystal structure without inverting the chirality, only the additional generators of the chirality-preserving Euclidean normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ should be used.

(2) $\mathcal{G}$ belongs to a pair of chiral space groups. Then its Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ consists only of proper motions, *i.e.* it likewise is a Sohncke space group. In that case, the symmetry groups of enantiomorphic crystals are enantimorphic space groups and, therefore, their coordinate descriptions cannot be mapped onto one another by symmetry operations from $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

Example for case (1)

The phosphorus atoms of NaP form helical chains with (slightly distorted) symmetry $\not{p}4_322$ (rod group of the molecules, not imposed by the space group; Schnering & Hönle, 1979). The chains wind round 2_1 axes parallel to **b** in the space group $\mathcal{G}=P2_12_12_1$. The Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is *Pmmm* with halved basis vectors (Table 3.5.2.4); the chirality-preserving Euclidean normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ is its noncentrosymmetric subgroup $P222$. The index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is 16 and shows the existence of 16 equivalent descriptions, namely of 8 enantiomorphic pairs. The index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ is 8. This corresponds to eight equivalent coordinate sets which can be obtained by application of the translations $0,0,0$; $\frac{1}{2},0,0$; $0,\frac{1}{2},0$; $0,0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$; $\frac{1}{2},0,\frac{1}{2}$; $0,\frac{1}{2},\frac{1}{2}$ and $\frac{1}{2},\frac{1}{2},\frac{1}{2}$. The remaining eight, with the opposite chirality, result from the same translations in addition to an inversion. The inversion converts the left-handed $\not{p}4_322$ helices to the enantiomorphic right-handed $\not{p}4_122$ helices. The chirality is a property of the polymeric $(P^-)_\infty$ ions. The space group $P2_12_12_1$ itself is not chiral, but it contains no symmetry operations that interconvert the enantiomeric ions; it is a Sohncke space group. The non-chiral space group $P2_12_12_1$ is compatible with either of the enantiomorphic forms of NaP.

Example for case (2)

Low-temperature quartz crystallizes either with symmetry $\mathcal{G}_1=P3_121$ (left-handed quartz) or $\mathcal{G}_2=P3_221$ (right-handed), which is a pair of enantiomorphic (chiral) space groups. Their Euclidean normalizers also form a pair of enantiomorphic space groups, namely $\mathcal{N}_{\mathcal{E}}(\mathcal{G}_1)=\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}_1)=$ $P6_222$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G}_2)=\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}_2)=P6_422$ with halved **c** vectors; they consist only of proper motions and thus are chirality preserving. The index of $P3_121$ in its Euclidean normalizer is 4, which means that there are four equivalent descriptions for left-handed quartz. They are mapped onto each other by the translation $0,0,\frac{1}{2}$ and the rotation $-x,-y,z$ (Table 3.5.2.5). The same applies to right-handed quartz. Left-handed quartz cannot be mapped onto right-handed quartz by the Euclidean normalizer. The four equivalent descriptions retain the chirality.

More details on Euclidean-equivalent point configurations and descriptions of crystal structures have been given by Fischer & Koch (1983) and Koch & Fischer (2006).

3.5.3.3. Equivalent lists of structure factors

All the different but equivalent descriptions of a crystal structure refer to different but equivalent lists of structure factors. These lists contain the same moduli of the structure factors $|F(\boldsymbol{h})|$, but they differ in their indices $\boldsymbol{h} = (h, k, l)$ and phases $\varphi(\boldsymbol{h})$.

In the previous section, the unit cell (basis and origin) of a space group $\mathcal{G}$ has been considered fixed, whereas the crystal structure or its enantiomorph was embedded into the pattern of symmetry elements at different but equivalent locations. In the present context, however, it is advantageous to regard the crystal structure as being fixed and to let $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ transform the basis and the origin with respect to which the crystal structure is described. This matches the usual approach to resolve the ambiguities in direct methods by fixing the origin and the absolute structure.

Each matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ representing an element of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ describes a unit-cell transformation of $\mathcal{G}$. According to Section 1.5.2 the following equations hold:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}'), = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}, \qquad \begin{pmatrix} \mathbf{a}^{*\prime} \\ \mathbf{b}^{*\prime} \\ \mathbf{c}^{*\prime} \end{pmatrix} = \boldsymbol{P}^{-1} \begin{pmatrix} \mathbf{a}^{*} \\ \mathbf{b}^{*} \\ \mathbf{c}^{*} \end{pmatrix}, \qquad \boldsymbol{h}' = \boldsymbol{hP}.$$

As a consequence, the phase $\varphi(\boldsymbol{h})$ of a given structure factor also changes into $\varphi'(\boldsymbol{h}') = \varphi(\boldsymbol{h}) - 2\pi\boldsymbol{hp}$.

Similar to equivalent descriptions of a crystal structure, it is possible to derive all equivalent lists of structure factors: The additional generators of $\mathcal{K}(\mathcal{G})$ are pure translations that leave the indices $\boldsymbol{h}$ of all structure factors unchanged but transform their phases according to $\varphi'(\boldsymbol{h}) = \varphi(\boldsymbol{h}) - 2\pi\boldsymbol{hp}$. Therefore, the origin for the description of the crystal structure may be fixed by appropriate restrictions of some phases. The number of these phases equals the number of additional generators of $\mathcal{K}(\mathcal{G})$, given in Tables 3.5.2.3, 3.5.2.4 or 3.5.2.5. These generators [together with the inversion that generates $\mathcal{L}(\mathcal{G})$, if present] also determine the parity classes of the structure factors and the ranges for the phase restrictions.

The inversion that generates $\mathcal{L}(\mathcal{G})$ changes the handedness of the coordinate system in direct space and in reciprocal space and, therefore, gives rise to different absolute crystal structures. The indices of a given structure factor change from $\boldsymbol{h}$ to $\boldsymbol{h}' = -\boldsymbol{h}$, whereas the phase is influenced only if the symmetry centre is not located at 0, 0, 0.

If no anomalous scattering is observed, Friedel's rule holds and the moduli of any two structure factors with indices $\boldsymbol{h}$ and $-\boldsymbol{h}$ are equal. As a consequence, different absolute crystal structures result in lists of structure factors and indices that differ only in their phases. Therefore, one phase may be restricted to an appropriate range of length π to fix the absolute structure. This is not possible if anomalous scattering has been observed.

If $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$, *i.e.* if $\mathcal{G}$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ belong to different Laue classes, the further generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ always change the orientation of the basis in direct and in reciprocal space. Therefore, the indices of the structure factors are permuted, but their phases are transformed only if $\boldsymbol{p} \neq \boldsymbol{o}$. The choice between these equivalent descriptions of the crystal structure is made when indexing the reflection pattern. In the case of anomalous scattering, the similar choice between the absolute structures is also combined with the indexing procedure.

Table 3.5.3.1
Changes of structure-factor phases for the equivalent descriptions of a crystal structure in *F*222

	$h+k+l=$			
*F*222	$4n$	$4n+2$	$4n+1$	$4n+3$
$t(0, 0, 0)$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$
$t(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$	$\varphi(\boldsymbol{h})$	$\pi + \varphi(\boldsymbol{h})$	$\frac{3}{2}\pi + \varphi(\boldsymbol{h})$	$\frac{1}{2}\pi + \varphi(\boldsymbol{h})$
$t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\pi + \varphi(\boldsymbol{h})$	$\pi + \varphi(\boldsymbol{h})$
$t(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$	$\varphi(\boldsymbol{h})$	$\pi + \varphi(\boldsymbol{h})$	$\frac{1}{2}\pi + \varphi(\boldsymbol{h})$	$\frac{3}{2}\pi + \varphi(\boldsymbol{h})$
$\bar{1}\ \ 0, 0, 0$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$
$\bar{1}\ \ \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$-\varphi(\boldsymbol{h})$	$\pi - \varphi(\boldsymbol{h})$	$\frac{1}{2}\pi - \varphi(\boldsymbol{h})$	$\frac{3}{2}\pi - \varphi(\boldsymbol{h})$
$\bar{1}\ \ \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$\pi - \varphi(\boldsymbol{h})$	$\pi - \varphi(\boldsymbol{h})$
$\bar{1}\ \ \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$	$-\varphi(\boldsymbol{h})$	$\pi - \varphi(\boldsymbol{h})$	$\frac{3}{2}\pi - \varphi(\boldsymbol{h})$	$\frac{1}{2}\pi - \varphi(\boldsymbol{h})$

Example

According to Table 3.5.2.4, eight equivalent descriptions exist for each crystal structure with symmetry *F*222. Four of them differ only by an origin shift and the other four are enantiomorphic to the first four. $t(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ transforms all phases according to $\varphi'(\boldsymbol{h}) = \varphi(\boldsymbol{h}) - (\pi/2)(h + k + l)$, which gives rise to four parity classes of structure factors: $h + k + l = 4n$, $4n + 1$, $4n + 2$ and $4n + 3$ (n integer). As $t(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ generates all additional translations of $\mathcal{K}(F222)$, restriction of one phase $\varphi(\boldsymbol{h}_1)$ to a range of length $\pi/2$ fixes the origin. Restriction of a second phase $\varphi(\boldsymbol{h}_2)$ to an appropriately chosen range of length π discriminates between pairs of enantiomorphic descriptions in the absence of anomalous scattering. For inversion through the origin $\bar{1}$ 0, 0, 0, the corresponding change of phases is $\varphi'(\boldsymbol{h}) = -\varphi(\boldsymbol{h})$. Table 3.5.3.1 shows, for structure factors from all parity classes, how their phases depend on the chosen description of the crystal structure. Only phases from parity classes $h + k + l = 4n + 1$ or $4n + 3$ determine the origin in a unique way. The phase $\varphi(\boldsymbol{h}_2)$ that fixes the absolute structure may be chosen from any parity class but the appropriate range for its restriction depends on the parity classes of $\varphi(\boldsymbol{h}_1)$ *and* $\varphi(\boldsymbol{h}_2)$ and, moreover, on the range chosen for $\varphi(\boldsymbol{h}_1)$. If, for instance, $\varphi(\boldsymbol{h}_1)$ with $h + k + l = 4n + 1$ is restricted to $\pi/2 \leq \varphi(\boldsymbol{h}_1) < \pi$, one of the following restrictions may be chosen for $\varphi(\boldsymbol{h}_2)$: $0 < \varphi(\boldsymbol{h}_2) < \pi$ for $h + k + l = 4n$; $-\pi/2 < \varphi(\boldsymbol{h}_2) < \pi/2$ for $h + k + l = 4n + 2$; $-\pi/4 < \varphi(\boldsymbol{h}_2) < 3\pi/4$ for $h + k + l = 4n + 1$; $-3\pi/4 < \varphi(\boldsymbol{h}_2) < \pi/4$ for $h + k + l = 4n + 3$. If, however, the phase $\varphi(\boldsymbol{h}_1)$ of the same first reflection was restricted to $-\pi/4 \leq \varphi(\boldsymbol{h}_1) < 3\pi/4$, the possible restrictions for the second phase change to: $0 < \varphi(\boldsymbol{h}_2) < \pi$ for $h + k + l = 4n$ or $4n + 2$; $-\pi/2 < \varphi(\boldsymbol{h}_2) < \pi/2$ for $h + k + l = 4n + 1$ or $4n + 3$ (for further details, *cf.* Koch, 1986).

3.5.3.4. Euclidean- and affine-equivalent sub- and supergroups

The Euclidean or affine normalizer of a space group $\mathcal{G}$ maps any subgroup or supergroup of $\mathcal{G}$ either onto itself or onto another subgroup or supergroup of $\mathcal{G}$. Accordingly, these normalizers define equivalence relationships on the sets of subgroups and supergroups of $\mathcal{G}$ (Koch, 1984*b*):

Two *subgroups* or *supergroups* 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 an element of the Euclidean (affine) normalizer of $\mathcal{G}$, *i.e.* if they are conjugate subgroups of the Euclidean (affine) normalizer.

In the following, the term 'equivalent subgroups (supergroups)' is used if a statement is true for Euclidean-equivalent *and* affine-equivalent subgroups (supergroups), and $\mathcal{N}(\mathcal{G})$ is used to designate the Euclidean as well as the affine normalizer.

The knowledge of Euclidean-equivalent subgroups is necessary in connection with the possible deformations of a crystal structure due to symmetry reduction. Affine-equivalent subgroups play an important role for the derivation and classification of black-and-white groups (magnetic groups) and of colour groups (*cf.* for example Schwarzenberger, 1984). Information on equivalent supergroups is useful for the determination of the idealized type of a crystal structure.

For any pair of space groups $\mathcal{G}$ and $\mathcal{H}$ with $\mathcal{H} < \mathcal{G}$, the relation between the two normalizers $\mathcal{N}(\mathcal{G})$ and $\mathcal{N}(\mathcal{H})$ controls the subgroups of $\mathcal{G}$ that are equivalent to $\mathcal{H}$ and the supergroups of $\mathcal{H}$ equivalent to $\mathcal{G}$. The intersection group of both normalizers, $\mathcal{M}(\mathcal{G}, \mathcal{H}) = \mathcal{N}(\mathcal{G}) \cap \mathcal{N}(\mathcal{H}) \geq \mathcal{H}$ may or may not coincide with $\mathcal{N}(\mathcal{G})$ and/or with $\mathcal{N}(\mathcal{H})$. The following two statements hold generally:

(i) The index i_g of $\mathcal{M}(\mathcal{G}, \mathcal{H})$ in $\mathcal{N}(\mathcal{G})$ equals the number of subgroups of $\mathcal{G}$ which are equivalent to $\mathcal{H}$. Each coset of $\mathcal{M}(\mathcal{G}, \mathcal{H})$ in $\mathcal{N}(\mathcal{G})$ maps $\mathcal{H}$ onto another equivalent subgroup of $\mathcal{G}$.

(ii) The index i_h of $\mathcal{M}(\mathcal{G}, \mathcal{H})$ in $\mathcal{N}(\mathcal{H})$ equals the number of supergroups of $\mathcal{H}$ equivalent to $\mathcal{G}$. Each coset of $\mathcal{M}(\mathcal{G}, \mathcal{H})$ in $\mathcal{N}(\mathcal{H})$ maps $\mathcal{G}$ onto another equivalent supergroup of $\mathcal{H}$.

Equivalent subgroups are *conjugate* in $\mathcal{G}$ if and only if $\mathcal{G} \cap \mathcal{N}(\mathcal{H}) \neq \mathcal{G}$. In this case, $\mathcal{G}$ contains elements not belonging to $\mathcal{N}(\mathcal{H})$ and the cosets of $\mathcal{G} \cap \mathcal{N}(\mathcal{H})$ in $\mathcal{G}$ refer to the different conjugate subgroups.

Examples

(1) $\mathcal{G} = Cmmm$ has four monoclinic subgroups of type $P2/m$ with the same orthorhombic metric and the same basis as $Cmmm$: $\mathcal{H}_1 = P2/m11$, $\mathcal{H}_2 = P12/m1$, $\mathcal{H}_3 = P112/m$ ($\bar{1}$ at $0,0,0$), $\mathcal{H}_4 = P112/m$ ($\bar{1}$ at $\frac{1}{4},\frac{1}{4},0$). According to Table 3.5.2.4, the Euclidean normalizer of $\mathcal{G}$ is $Pmmm$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$. Because of the orthorhombic metric of all four subgroups, their Euclidean normalizers $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_1)$, $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_2)$, $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_3)$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_4)$ are enhanced in comparison with the general case and coincide with $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$. Hence, no two of the four subgroups are Euclidean-equivalent.

(2) $\mathcal{G} = I\bar{4}m2$ $(\mathbf{a}, \mathbf{b}, \mathbf{c})$, $\mathcal{H} = P\bar{4}$ $(\mathbf{a}, \mathbf{b}, \mathbf{c})$.
$\mathcal{N}(\mathcal{G}) = I4/mmm$ $(\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ is a supergroup of index 2 of $\mathcal{N}(\mathcal{H}) = P4/mmm$ $(\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}) = \mathcal{M}(I\bar{4}m2, P\bar{4})$. Therefore, $I\bar{4}m2$ has two equivalent subgroups $P\bar{4}$ that are mapped onto one another by a centring translation of $\mathcal{N}(\mathcal{G})$, *e.g.* by $t(0, \frac{1}{2}, \frac{1}{4})$. Both subgroups are not conjugate in $I\bar{4}m2$ because $\mathcal{G} \cap \mathcal{N}(\mathcal{H})$ equals $\mathcal{G}$. As $\mathcal{N}(\mathcal{H})$ coincides with $\mathcal{M}(\mathcal{G}, \mathcal{H})$, no further supergroups of $P\bar{4}$ equivalent to $I\bar{4}m2$ exist.

(3) $\mathcal{G} = Fm\bar{3}$ $(\mathbf{a}, \mathbf{b}, \mathbf{c})$, $\mathcal{H} = F23$ $(\mathbf{a}, \mathbf{b}, \mathbf{c})$.
$\mathcal{N}(\mathcal{H}) = Im\bar{3}m$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ is a supergroup of index 2 of $\mathcal{N}(\mathcal{G}) = Pm\bar{3}m$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}) = \mathcal{M}(Fm\bar{3}, F23)$. Therefore, $F23$ has two equivalent supergroups $Fm\bar{3}$ that differ in their locations with site symmetry $m\bar{3}$ by a centring translation of $Im\bar{3}m$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$, *e.g.* by $t(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. As $\mathcal{N}(\mathcal{G})$ coincides with $\mathcal{M}(\mathcal{G}, \mathcal{H})$, no further subgroups of $Fm\bar{3}$ equivalent to $F23$ exist.

(4) $\mathcal{G} = Pmma$ $(\mathbf{a}, \mathbf{b}, \mathbf{c})$, $\mathcal{H} = Pmmn$ $(\mathbf{a}, 2\mathbf{b}, \mathbf{c})$.
The intersection of $\mathcal{N}_{\mathcal{A}}(Pmma) = Pmmm$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ and $\mathcal{N}_{\mathcal{A}}(Pmmn) = P4/mmm$ $(\frac{1}{2}\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c})$ is the group $\mathcal{M}(Pmma, Pmmn) = Pmmm$ $(\frac{1}{2}\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c})$, which is a proper subgroup of both normalizers. As i_g equals 2, $Pmma$ has two affine-equivalent subgroups of type $Pmmn$ that are mapped onto each other by the additional translation $t(0, \frac{1}{2}, 0)$ of the normalizer of $\mathcal{G}$. As i_h also equals 2, $Pmmn$ has two affine-equivalent supergroups, $Pmma$ and $Pmmb$, that are mapped onto each other, *e.g.* by the affine 'reflection' at a diagonal 'mirror plane' of $\mathcal{N}_{\mathcal{A}}(\mathcal{H})$.

3.5.3.5. Reduction of the parameter regions to be considered for geometrical studies of point configurations

Each point configuration with space-group symmetry $\mathcal{G}$ may be described by its metrical and coordinate parameters. To cover all point configurations belonging to a certain space-group type exactly once, the metrical parameters of $\mathcal{G}$ have to be varied without restrictions, whereas the coordinate parameters x, y and z must be restricted to one asymmetric unit of $\mathcal{G}$. For the study of the geometrical properties of point configurations (*e.g.* sphere-packing conditions or types of Dirichlet domains *etc.*), the Euclidean normalizers (*cf. e.g.* Laves, 1931; Fischer, 1971, 1991; Koch, 1984*a*) as well as the affine normalizers (*cf.* Fischer, 1968) of the space groups allow a further reduction of the parameter regions that have to be considered.

Examples

(1) $\mathcal{G} = P4/m$ with asymmetric unit $0 \leq x \leq \frac{1}{2}$, $0 < y < \frac{1}{2}$, $0 \leq z \leq \frac{1}{2}$: A geometrical consideration may be restricted to one asymmetric unit of $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = \mathcal{N}_{\mathcal{A}}(\mathcal{G}) = P4/mmm$ $(\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$, *i.e.* to the region $0 \leq x \leq \frac{1}{2}$, $y \leq \min(x, \frac{1}{2} - x)$, $0 \leq z \leq \frac{1}{4}$. All metrical parameters are unrestricted.

(2) $\mathcal{G} = P4$ with asymmetric unit $0 \leq x \leq \frac{1}{2}$, $0 < y < \frac{1}{2}$, $0 \leq z < 1$: The normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = \mathcal{N}_{\mathcal{A}}(\mathcal{G}) = P^14/mmm$ $(\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c})$ restricts the parameter region to be considered to $0 \leq x \leq \frac{1}{2}$, $y \leq \min(x, \frac{1}{2} - x)$, $z = 0$. Again, no restriction exists for the metrical parameters.

(3) $\mathcal{G} = Pmmm$ with asymmetric unit $0 \leq x \leq \frac{1}{2}$, $0 \leq y \leq \frac{1}{2}$, $0 \leq z \leq \frac{1}{2}$: The Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = Pmmm$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ reduces the parameter region to be considered to $0 \leq x \leq \frac{1}{4}$, $0 \leq y \leq \frac{1}{4}$, $0 \leq z \leq \frac{1}{4}$. All metrical parameters are unrestricted. The affine normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{G}) = Pm\bar{3}m$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ enables a further reduction of the parameter region that has to be studied. For this, two different possibilities exist:
  (i) the metrical parameters remain unrestricted but the coordinate parameters are limited to one asymmetric unit of $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$, *i.e.* to $0 \leq x \leq \frac{1}{4}$, $0 \leq y \leq x$, $0 \leq z \leq y$;
  (ii) the coordinate parameters are not further restricted, but the metrical parameters have to obey *e.g.* the relation $a \leq b \leq c$, *i.e.* $a/c \leq b/c \leq 1$.

(4) $\mathcal{G} = P112/m$ with asymmetric unit $0 \leq x < 1$, $0 \leq y \leq \frac{1}{2}$, $0 \leq z \leq \frac{1}{2}$. The Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = P112/m$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ reduces the region that has to be considered for the coordinate parameters to $0 \leq x < \frac{1}{2}$, $0 \leq y \leq \frac{1}{4}$, $0 \leq z \leq \frac{1}{4}$, but it does not impose restrictions on the metrical parameters. These may be restricted, however, to the range $a/b \leq 1$ and $0 \leq 2\cos\gamma \leq -a/b$ (as shown in Fig. 3.5.2.1) by means of the affine normalizer $\mathcal{N}_{\mathcal{A}}(P112/m)$.

references