

3.5. Normalizers of space groups and their use in crystallography

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3.5.1. Introduction and definitions

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3.5.1.1. Introduction

The mathematical concept of normalizers forms the common basis for the solution of several crystallographic problems:

It is generally known, for instance, that the coordinate description of a crystal structure trivially depends on the coordinate system used for the description, *i.e.* on the setting of the space group and the site symmetry of the origin. It is less well known, however, that for most crystal structures there exist several different but equivalent coordinate descriptions, even if the space-group setting and the site symmetry of the origin are unchanged. The number of such descriptions varies between 1 and 24 and depends only on the type of the Euclidean normalizer of the corresponding space group. In principle, none of these descriptions stands out against the others.

In crystal-structure determination with direct methods, the phases of some suitably chosen structure factors have to be restricted to certain values or to certain ranges in order to specify the origin and the enantiomorph. The information necessary for a correct selection of such phases and for their appropriate restrictions follows directly from the Euclidean normalizer of the space group. Similar examples are the positioning of the first atom(s) within an asymmetric unit when using trial-and-error or Patterson methods, the choice of a basis system for indexing the reflections of a diffraction pattern or the indexing of the first morphological face(s) of a crystal.

For the following problems, normalizers also play an important role: They supply information on the interchangeability of Wyckoff positions and their assignment to Wyckoff sets (*cf.* Section 1.4.4 and Chapter 3.4), needed *e.g.* for the definition of lattice complexes. They are important for the comparison of crystal structures, for their assignment to structure types and for the choice of a standard description for each crystal structure (Parthé & Gelato, 1984, 1985). They allow the derivation of ‘privileged origins’ for each space group (Burzlaff & Zimmermann, 1980) and facilitate the complete deduction of subgroups and supergroups of a crystallographic group. They enable an easy classification of magnetic (black–white or Shubnikov) space groups and of colour space groups. They may also be used to reduce the parameter range in the study of geometrical properties of point configurations, *e.g.* their eigensymmetry or their sphere packings and Dirichlet partitions (*cf. e.g.* Koch, 1984*a*).

In the past, most of these problems have been treated by crystallographers without the aid of normalizers, but the use of normalizers simplifies the solution of all these problems and clarifies the common background (for references, see Fischer & Koch, 1983).

3.5.1.2. Definitions

Any pair, consisting of a group \mathcal{G} and one of its supergroups \mathcal{S} , is uniquely related to a third intermediate group $\mathcal{N}_{\mathcal{S}}(\mathcal{G})$, called the *normalizer of \mathcal{G} with respect to \mathcal{S}* . $\mathcal{N}_{\mathcal{S}}(\mathcal{G})$ is defined as the set of all

elements $s \in \mathcal{S}$ that map \mathcal{G} onto itself by conjugation (*cf.* Section 1.1.8):

$$\mathcal{N}_{\mathcal{S}}(\mathcal{G}) := \{s \in \mathcal{S} \mid s^{-1}\mathcal{G}s = \mathcal{G}\}.$$

The normalizer $\mathcal{N}_{\mathcal{S}}(\mathcal{G})$ may coincide either with \mathcal{G} or with \mathcal{S} or it may be a proper intermediate group. In any case, \mathcal{G} is a normal subgroup of its normalizer.

For most crystallographic problems, three kinds of normalizers are of special interest:

- (i) The normalizer of a space group (plane group) \mathcal{G} with respect to the group \mathcal{E} of all Euclidean mappings (motions, isometries) in \mathbb{E}^3 (\mathbb{E}^2), called the *Euclidean normalizer of \mathcal{G}* :

$$\mathcal{N}_{\mathcal{E}}(\mathcal{G}) := \{s \in \mathcal{E} \mid s^{-1}\mathcal{G}s = \mathcal{G}\}.$$

- (ii) The normalizer of a space group (plane group) \mathcal{G} with respect to the group \mathcal{A} of all affine mappings in \mathbb{E}^3 (\mathbb{E}^2), called the *affine normalizer of \mathcal{G}* :

$$\mathcal{N}_{\mathcal{A}}(\mathcal{G}) := \{s \in \mathcal{A} \mid s^{-1}\mathcal{G}s = \mathcal{G}\}.$$

- (iii) The normalizer of a space group \mathcal{G} with respect to the group \mathcal{E}^+ of all chirality-preserving Euclidean mappings in \mathbb{E}^3 , *i.e.* of all translations and proper rotations (including screw rotations), but excluding symmetry operations of the second kind (*viz.* inversions, reflections, glide reflections and rotoinversions). We call it the *chirality-preserving Euclidean normalizer of \mathcal{G}* :

$$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}) := \{s \in \mathcal{E}^+ \mid s^{-1}\mathcal{G}s = \mathcal{G}\}.$$

$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ exists only if \mathcal{G} is a Sohncke space group. The 65 *Sohncke space-group types* are those space-group types that have no symmetry operations of the second kind (Flack, 2003).¹ They include the eleven pairs of types of enantiomorphic space groups; these eleven pairs are the only ones where the space groups themselves are chiral, *i.e.* which have an Euclidean normalizer containing only isometries of the first kind. The space groups of the remaining 43 Sohncke types are not chiral but do allow chiral crystal structures. A rigid object (or spatial arrangement of points or atoms) is *chiral* if it is nonsuperposable by pure rotation or translation on its image formed by inversion through a point. A chiral crystal structure is compatible only with a Sohncke space group.

The Euclidean normalizers of the space groups were first derived by Hirshfeld (1968) under the name *Cheshire groups*. They have been tabulated in more detail by Gubler (1982*a,b*) and Fischer & Koch (1983). The Euclidean normalizers of triclinic and monoclinic space groups with specialized metric of the lattice were determined by Koch & Müller (1990). The affine normalizers of the space groups have been listed by Burzlaff & Zimmermann (1980), Billiet *et al.* (1982) and Gubler (1982*a,b*). They were also used for the derivation of Wyckoff sets and the

¹ Sohncke (1879) was the first to derive the 65 space-group types having only symmetry operations of the first kind (translations, rotations and screw rotations). As proposed by Flack (2003), these are called the 65 Sohncke space-group types.

definition of lattice complexes by Koch & Fischer (1975), even though there the automorphism groups of the space groups were tabulated instead of their affine normalizers. The chirality-preserving Euclidean normalizers are tabulated in this volume for the first time.

3.5.2. Euclidean and affine normalizers of plane groups and space groups

BY E. KOCH, W. FISCHER AND U. MÜLLER

3.5.2.1. Euclidean normalizers of plane groups and space groups

Since each symmetry operation of the Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ maps the space group \mathcal{G} onto itself, it also maps the set of all symmetry elements of \mathcal{G} onto itself. Therefore, the Euclidean normalizer of a space group can be interpreted as the group of motions that maps the pattern of symmetry elements of the space group onto itself, *i.e.* as the 'symmetry of the symmetry pattern'.

For most space (plane) groups, the Euclidean normalizers are space (plane) groups again. Exceptions are those groups where origins are not fully fixed by symmetry, *i.e.* all space groups of the geometrical crystal classes 1, m , 2, $2mm$, 3, $3m$, 4, $4mm$, 6 and $6mm$, and all plane groups of the geometrical crystal classes 1 and m . The Euclidean normalizer of each such group contains continuous translations (*i.e.* translations of infinitesimal length) in one, two or three independent lattice directions and, therefore, is not a space (plane) group but a supergroup of a space (plane) group.

If one regards a certain type of space (plane) group, usually the Euclidean normalizers of all corresponding groups belong also to only one type of normalizer. This is true for all cubic, hexagonal, trigonal and tetragonal space groups (hexagonal and square plane groups) and, in addition, for 21 types of orthorhombic space group (4 types of rectangular plane group), *e.g.* for $Pnma$.

In contrast to this, the Euclidean normalizer of a space (plane) group belonging to one of the other 38 orthorhombic (3 rectangular) types may interchange two or even three lattice directions if the corresponding basis vectors have equal length (example: $Pnmm$ with $a = b$). Then, the Euclidean normalizer of this group belongs to the tetragonal (square) or even to the cubic crystal system, whereas another space (plane) group of the same type but with general metric has an orthorhombic (rectangular) Euclidean normalizer.

For each space (plane)-group type belonging to the monoclinic (oblique) or triclinic system, there also exist groups with specialized metric that have Euclidean normalizers of higher symmetry than for the general case (*cf.* Koch & Müller, 1990). The description of these special cases, however, is by far more complicated than for the orthorhombic system.

The symmetry of the Euclidean normalizer of a monoclinic (oblique) space (plane) group depends only on two metrical parameters. A clear presentation of all cases with specialized metric may be achieved by choosing the cosine of the monoclinic angle and the related axial ratio as parameters. To cover all different metrical situations exactly once, not all pairs of parameter values are allowed for a given type of space (plane) group, but one has to restrict the study to a certain parameter range depending on the type, the setting and the cell choice of the space (plane) group. Parthé & Gelato (1985) have discussed in detail such parameter regions for the first setting of the monoclinic space groups. Figs. 3.5.2.1 to 3.5.2.4 are based on these studies.

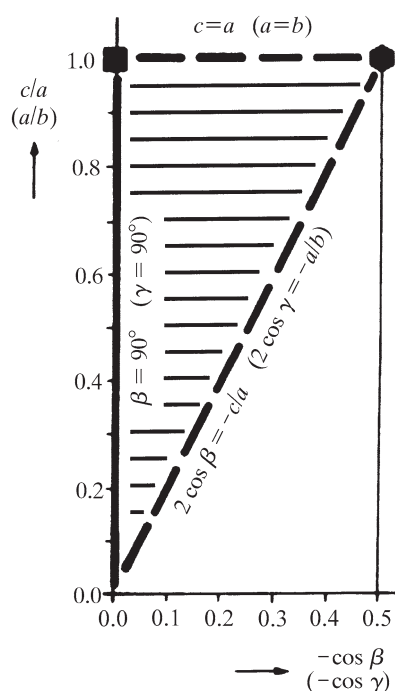


Figure 3.5.2.1

Parameter range for space groups of types $P2$, $P2_1$, Pm , $P2/m$ and $P2_1/m$ (plane groups of types $p1$ and $p2$). The information in parentheses refers to unique axis c .

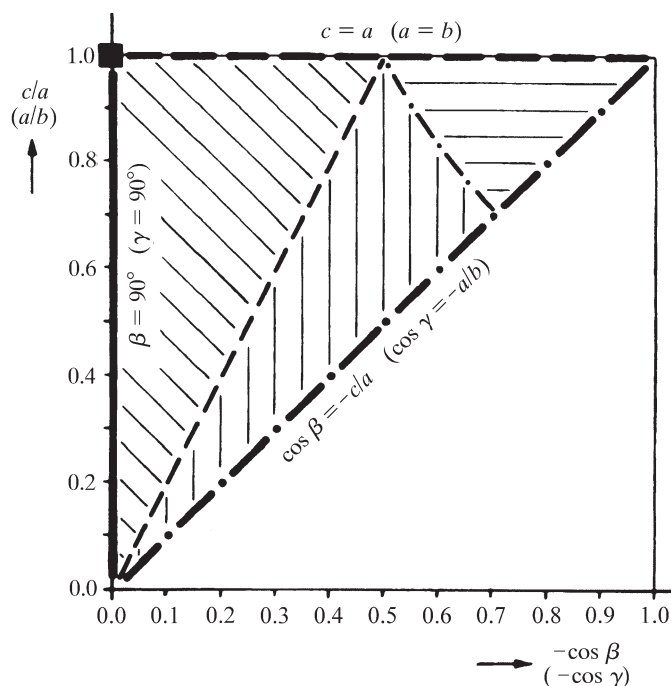
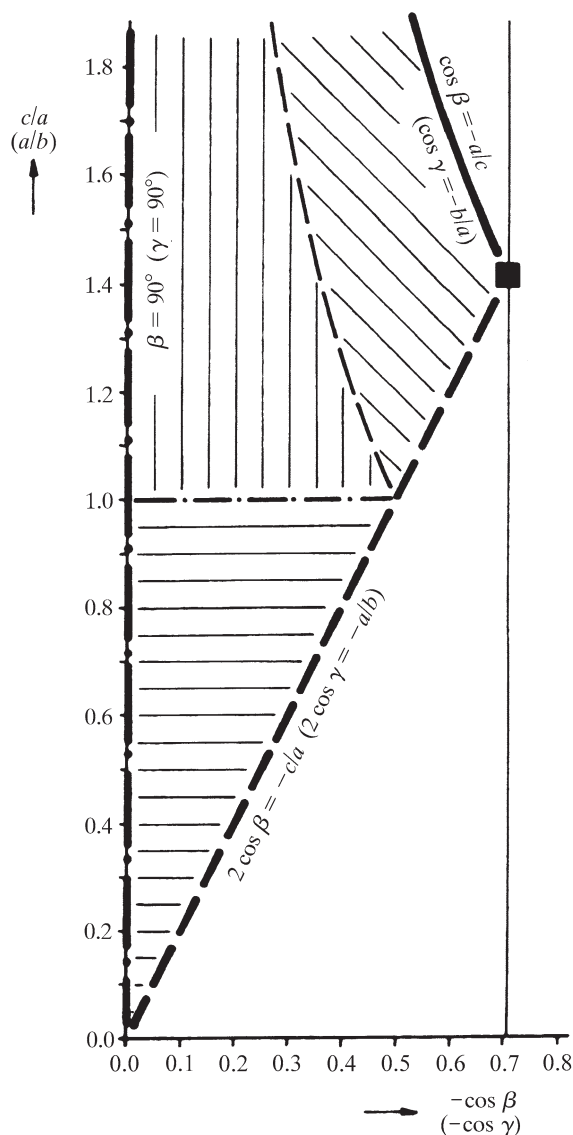


Figure 3.5.2.2

Parameter range for space groups of types $C2$, Pc , Cm , Cc , $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$. They refer to the following settings:
 unique axis b , cell choice 2: $P1n1$, $I12/n1$, $P12_1/n1$;
 unique axis b , cell choice 3: $I121$, $I1m1$, $I1a1$, $I12/m1$, $I12/a1$;
 unique axis c , cell choice 2: $P11n$, $P112/n$, $P112_1/n$;
 unique axis c , cell choice 3: $I112$, $I11m$, $I11b$, $I112/m$, $I112/b$.
 The information in parentheses refers to unique axis c .

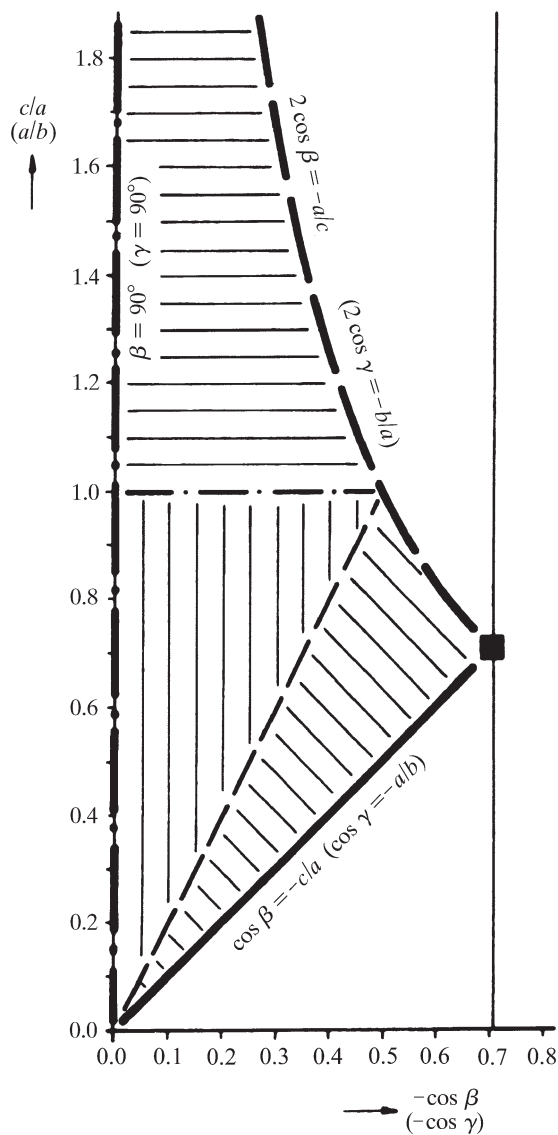
Fig. 3.5.2.1 shows a suitably chosen parameter region for the five space-group types $P2$, $P2_1$, Pm , $P2/m$ and $P2_1/m$ and for the plane-group types $p1$ and $p2$. Each such space (plane) group with general metric may be uniquely assigned to an inner point of this region and any metrical specialization corresponds either to one of the three boundary lines or to one of their points of inter-


Figure 3.5.2.3

Parameter range for space groups of types $C2$, Pc , Cm , Cc , $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$:

- unique axis b , cell choice 1: $P1c1$, $P12/c1$, $P12_1/c1$;
- unique axis b , cell choice 2: $A121$, $A1m1$, $A1n1$, $A12/m1$, $A12/n1$;
- unique axis c , cell choice 1: $P11a$, $P112/a$, $P112_1/a$;
- unique axis c , cell choice 2: $B112$, $B11m$, $B11n$, $B112/m$, $B112/n$.

The information in parentheses refers to unique axis c .


Figure 3.5.2.4

Parameter range for space groups of types $C2$, Pc , Cm , Cc , $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$:

- unique axis b , cell choice 1: $C121$, $C1m1$, $C1c1$, $C12/m1$, $C12/c1$;
- unique axis b , cell choice 3: $P1a1$, $P12/a1$, $P12_1/a1$, $C12/c1$;
- unique axis c , cell choice 1: $A112$, $A11m$, $A11a$, $A112/m$, $A112/a$;
- unique axis c , cell choice 3: $P11b$, $P112/b$, $P112_1/b$, $A112/a$.

The information in parentheses refers to unique axis c .

section and gives rise to a symmetry enhancement of the respective Euclidean normalizer.

For each of the other eight types of monoclinic space groups, *i.e.* $C2$, Pc , Cm , Cc , $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$, and for each setting three possibilities of cell choice are listed in Chapter 2.3, which can be distinguished by different space-group symbols (example: $C12/m1$, $A12/m1$, $I12/m1$, $A112/m$, $B112/m$, $I112/m$). For each setting, there exist two ways to choose a suitable range for the metrical parameters such that each group corresponds to exactly one point:

- (i) One arbitrarily restricts oneself to cell choice 1, 2 or 3. Then, the suitable parameter range (displayed in one of the Figs. 3.5.2.2, 3.5.2.3 or 3.5.2.4) is larger than the range shown in Fig. 3.5.2.1 because, in contrast to the space-group types discussed above, some of the possible metrical specializations do not give rise to any symmetry enhancement of the Euclidean normalizers. These special metrical cases refer to the light lines subdividing the parameter regions of Figs. 3.5.2.2 to

3.5.2.4. Again, all inner points of these regions correspond to space groups with Euclidean normalizers without enhanced symmetry, and all points on the heavy-line boundaries refer to space groups, the Euclidean normalizers of which show symmetry enhancement.

- (ii) For all types of monoclinic space groups, one regards only the small parameter region shown in Fig. 3.5.2.1, but in return takes into consideration all three possibilities for the cell choice. Then, however, not all boundaries of this small parameter region correspond to Euclidean normalizers with enhanced symmetry. (Similar considerations are true for oblique plane groups.)

For triclinic space groups, five metrical parameters are necessary and, therefore, it is impossible to describe the special metrical cases in an analogous way.

In general, between a space group (or plane group) \mathcal{G} and its Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$, two uniquely defined intermediate groups $\mathcal{K}(\mathcal{G})$ and $\mathcal{L}(\mathcal{G})$ exist, such that

3.5. NORMALIZERS OF SPACE GROUPS

Table 3.5.2.1

Euclidean normalizers of the plane groups

For the restrictions of the cell metric of the two oblique plane groups see text and Fig. 3.5.2.3.

Plane group \mathcal{G}		Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$			Index of \mathcal{G} in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$	
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Twofold rotation		Further generators
1	$p1$	General	p^22	$\varepsilon_1 \mathbf{a}, \varepsilon_2 \mathbf{b}$	$r, 0; 0, s$	$-x, -y$		$\infty^2 \cdot 2 \cdot 1$
		$a < b, \gamma = 90^\circ$	p^22mm	$\varepsilon_1 \mathbf{a}, \varepsilon_2 \mathbf{b}$	$r, 0; 0, s$	$-x, -y$	$-x, y$	$\infty^2 \cdot 2 \cdot 2$
		$2 \cos \gamma = -a/b, 90^\circ < \gamma < 120^\circ$	c^22mm	$\varepsilon_1 \mathbf{a}, \varepsilon_2 (\frac{1}{2}\mathbf{a} + \mathbf{b})$	$r, 0; 0, s$	$-x, -y$	$x - y, -y$	$\infty^2 \cdot 2 \cdot 2$
		$a = b, 90^\circ < \gamma < 120^\circ$	c^22mm	$\varepsilon_1(\mathbf{a} - \mathbf{b}), \varepsilon_2(\mathbf{a} + \mathbf{b})$	$r, 0; 0, s$	$-x, -y$	y, x	$\infty^2 \cdot 2 \cdot 2$
		$a = b, \gamma = 90^\circ$	p^24mm	$\varepsilon \mathbf{a}, \varepsilon \mathbf{b}$	$r, 0; 0, s$	$-x, -y$	$-x, y; y, x$	$\infty^2 \cdot 2 \cdot 4$
		$a = b, \gamma = 120^\circ$	p^26mm	$\varepsilon \mathbf{a}, \varepsilon \mathbf{b}$	$r, 0; 0, s$	$-x, -y$	$y, x; x, x - y$	$\infty^2 \cdot 2 \cdot 6$
2	$p2$	General	$p2$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a < b, \gamma = 90^\circ$	$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$-x, y$	$4 \cdot 1 \cdot 2$
		$2 \cos \gamma = -a/b, 90^\circ < \gamma < 120^\circ$	$c2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a} + \mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$x - y, -y$	$4 \cdot 1 \cdot 2$
		$a = b, 90^\circ < \gamma < 120^\circ$	$c2mm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b})$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		y, x	$4 \cdot 1 \cdot 2$
		$a = b, \gamma = 90^\circ$	$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$-x, y; y, x$	$4 \cdot 1 \cdot 4$
		$a = b, \gamma = 120^\circ$	$p6mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$y, x; x, x - y$	$4 \cdot 1 \cdot 6$
3	$p1m1$	$a \neq b$ $a = b$	p^12mm	$\frac{1}{2}\mathbf{a}, \varepsilon \mathbf{b}$	$\frac{1}{2}, 0; 0, s$	$-x, -y$		$(2 \cdot \infty) \cdot 2 \cdot 1$
4	$p1g1$		p^12mm	$\frac{1}{2}\mathbf{a}, \varepsilon \mathbf{b}$	$\frac{1}{2}, 0; 0, s$	$-x, -y$		$(2 \cdot \infty) \cdot 2 \cdot 1$
5	$c1m1$		p^12mm	$\frac{1}{2}\mathbf{a}, \varepsilon \mathbf{b}$	$0, s$	$-x, -y$		$\infty \cdot 2 \cdot 1$
6	$p2mm$		$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		y, x	$4 \cdot 1 \cdot 1$
			$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$			$4 \cdot 1 \cdot 2$
7	$p2mg$		$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
8	$p2gg$		$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
			$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		y, x	$4 \cdot 1 \cdot 2$
9	$c2mm$		$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0$			$2 \cdot 1 \cdot 1$
		$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0$		y, x	$2 \cdot 1 \cdot 2$	
10	$p4$		$p4mm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b})$	$\frac{1}{2}, \frac{1}{2}$		y, x	$2 \cdot 1 \cdot 2$
11	$p4mm$		$p4mm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b})$	$\frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
12	$p4gm$		$p4mm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b})$	$\frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
13	$p3$		$p6mm$	$\frac{1}{3}(2\mathbf{a} + \mathbf{b}), \frac{1}{3}(-\mathbf{a} + \mathbf{b})$	$\frac{2}{3}, \frac{1}{3}$	$-x, -y$	y, x	$3 \cdot 2 \cdot 2$
14	$p3m1$		$p6mm$	$\frac{1}{3}(2\mathbf{a} + \mathbf{b}), \frac{1}{3}(-\mathbf{a} + \mathbf{b})$	$\frac{2}{3}, \frac{1}{3}$	$-x, -y$		$3 \cdot 2 \cdot 1$
15	$p31m$		$p6mm$	\mathbf{a}, \mathbf{b}		$-x, -y$		$1 \cdot 2 \cdot 1$
16	$p6$		$p6mm$	\mathbf{a}, \mathbf{b}			y, x	$1 \cdot 1 \cdot 2$
17	$p6mm$		$p6mm$	\mathbf{a}, \mathbf{b}				$1 \cdot 1 \cdot 1$

$$\mathcal{G} \leq \mathcal{K}(\mathcal{G}) \leq \mathcal{L}(\mathcal{G}) \leq \mathcal{N}_{\mathcal{E}}(\mathcal{G})$$

holds. $\mathcal{K}(\mathcal{G})$ is that *klassengleiche* supergroup of \mathcal{G} that is at the same time a *translationengleiche* subgroup of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$. It is well defined according to the theorem of Hermann (1929). The group $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{K}(\mathcal{G})$ only if \mathcal{G} is noncentrosymmetric but $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is centrosymmetric; then $\mathcal{L}(\mathcal{G})$ is that centrosymmetric supergroup of $\mathcal{K}(\mathcal{G})$ of index 2 that is again a subgroup of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$. It belongs to the Laue class of \mathcal{G} . If $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is noncentrosymmetric, an intermediate group $\mathcal{L}(\mathcal{G})$ cannot exist.

The chirality-preserving Euclidean normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ of a Sohncke space group \mathcal{G} is the unique noncentrosymmetric subgroup of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ which is a supergroup of $\mathcal{K}(\mathcal{G})$:

$$\mathcal{G} \leq \mathcal{K}(\mathcal{G}) \leq \mathcal{N}_{\mathcal{E}^+}(\mathcal{G}) \leq \mathcal{N}_{\mathcal{E}}(\mathcal{G}).$$

If $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is centrosymmetric, $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ is a subgroup of index 2 of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$. If $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is noncentrosymmetric, $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ are identical.

With the aid of its chirality-preserving Euclidean normalizer it is possible to determine all equivalent sets of coordinates of a chiral crystal structure, excluding the opposite enantiomorph (*cf.* Section 3.5.3.2).

The groups $\mathcal{K}(\mathcal{G})$ and $\mathcal{L}(\mathcal{G})$ are of special interest in connection with direct methods for structure determination: they cause the

parity classes of reflections; $\mathcal{K}(\mathcal{G})$ defines the permissible origin shifts and the parameter ranges for the phase restrictions in the specification of the origin; and $\mathcal{L}(\mathcal{G})$ gives information on possible phase restrictions for the selection of the enantiomorph. For any space (plane) group \mathcal{G} , the translation subgroups of $\mathcal{K}(\mathcal{G})$, $\mathcal{L}(\mathcal{G})$, $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and even $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ coincide.

The Euclidean normalizers of the plane groups are listed in Table 3.5.2.1, those of triclinic space groups in Table 3.5.2.2. The Euclidean and the chirality-preserving Euclidean normalizers of monoclinic and orthorhombic space groups are in Tables 3.5.2.3 and 3.5.2.4, those of all other space groups in Table 3.5.2.5. Herein all settings and choices of cell and origin as tabulated in Chapters 2.2 and 2.3 are taken into account and, in addition, all metrical specializations giving rise to Euclidean normalizers with enhanced symmetry. Each setting, cell choice, origin or metrical specialization corresponds to one line in the tables. (Exceptions are some orthorhombic space groups with tetragonal metric: if $a = b$ as well as $b = c$ and $c = a$ give rise to a symmetry enhancement of the Euclidean normalizer, only the case $a = b$ is listed in Table 3.5.2.4.)

The first column of Tables 3.5.2.1, 3.5.2.3, 3.5.2.4 and 3.5.2.5 shows the number of the plane group or space group, and the second column shows its Hermann–Mauguin symbol together with information on the setting, cell choice and origin, if neces-

Table 3.5.2.2

Euclidean normalizers of the triclinic space groups

Basis vectors of the Euclidean normalizers ($\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ refer to the possibly centred conventional unit cell for the respective Bravais lattice): $P1: \varepsilon\mathbf{a}_c, \varepsilon\mathbf{b}_c, \varepsilon\mathbf{c}_c$; $P\bar{1}: \frac{1}{2}\mathbf{a}_c, \frac{1}{2}\mathbf{b}_c, \frac{1}{2}\mathbf{c}_c$.

Bravais type	Euclidean normalizer $\mathcal{N}_\varepsilon(\mathcal{G})$ of	
	$P1$ (1)	$P\bar{1}$ (2)
aP	$P^3\bar{1}$	$P\bar{1}$
mP	P^32/m	$P2/m$
mA	P^32/m	$A2/m$
oP	P^3mmm	$Pmmm$
oC	P^3mmm	$Cmmm$
oF	P^3mmm	$Fmmm$
oI	P^3mmm	$Immm$
tP	P^34/mmm	$P4/mmm$
tI	P^34/mmm	$I4/mmm$
hP	P^36/mmm	$P6/mmm$
hR	$P^3\bar{3}m1$	$R\bar{3}m$
cP	$P^3m\bar{3}m$	$Pm\bar{3}m$
cF	$P^3m\bar{3}m$	$Fm\bar{3}m$
cI	$P^3m\bar{3}m$	$Im\bar{3}m$

sary. Special metrical conditions affecting the Euclidean normalizer are tabulated in the third column of Tables 3.5.2.1, 3.5.2.3 and 3.5.2.4. The term ‘general’ means that only the general metrical conditions for the respective crystal system are valid. In Table 3.5.2.5, a corresponding column is superfluous because here a metrical specialization of the space group does not influence the type of the Euclidean normalizer.

The Euclidean normalizer of the space (plane) group is identified in the fourth column of Tables 3.5.2.3 and 3.5.2.4 (3.5.2.1) or in the third column of Table 3.5.2.5. As Euclidean normalizers are groups of motions, they can normally be designated by Hermann–Mauguin symbols. If, however, the origin of the space (plane) group is not fixed by symmetry (examples: $P4, P1m1, P1$), the Euclidean normalizer contains continuous translations in one, two or three (one or two) independent directions. In these cases, P^1, B^1, C^1, P^2 or P^3 (p^1, c^1, p^2), respectively, are used instead of the Bravais letter.² The setting and origin choice for the Euclidean normalizers are indicated as for space groups. In a few cases, origin choices not tabulated in Chapter 2.3 or nonconventional settings like $Bmmm$ instead of $Cmmm$ are needed.

In the next column, the basis of $\mathcal{N}_\varepsilon(\mathcal{G})$ is described in terms of the basis of \mathcal{G} . A factor ε is used to indicate continuous translations.

The following three columns specify the set of additional symmetry operations that generate $\mathcal{K}(\mathcal{G})$, $\mathcal{L}(\mathcal{G})$ and $\mathcal{N}_\varepsilon(\mathcal{G})$ or $\mathcal{N}_{\varepsilon^+}(\mathcal{G})$ successively from the space group \mathcal{G} . The first of them shows the vector components of the additional translations generating $\mathcal{K}(\mathcal{G})$ from \mathcal{G} ; components referring to continuous translations are labelled r, s and t . If $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{K}(\mathcal{G})$, *i.e.* if \mathcal{G} is noncentrosymmetric and $\mathcal{N}_\varepsilon(\mathcal{G})$ is centrosymmetric, the position of the additional centre of inversion is given in the second of these columns. The respective inversion generates $\mathcal{L}(\mathcal{G})$ from $\mathcal{K}(\mathcal{G})$. (For plane groups, additional twofold rotations play the role of these inversions.) $\mathcal{L}(\mathcal{G})$, however, is undefined for $\mathcal{N}_{\varepsilon^+}(\mathcal{G})$ and also if $\mathcal{N}_\varepsilon(\mathcal{G})$ is noncentrosymmetric; this fact is indicated by a slash. The last of these columns contains entries only if \mathcal{G} belongs to a different Laue class than $\mathcal{N}_\varepsilon(\mathcal{G})$ or $\mathcal{N}_{\varepsilon^+}(\mathcal{G})$.

The corresponding additional generators are listed as coordinate triplets.

In the last column, the subgroup index of \mathcal{G} in $\mathcal{N}_\varepsilon(\mathcal{G})$ is specified as the product $k_g l_k n_l$, where k_g means the index of \mathcal{G} in $\mathcal{K}(\mathcal{G})$, l_k the index of $\mathcal{K}(\mathcal{G})$ in $\mathcal{L}(\mathcal{G})$ and n_l the index of $\mathcal{L}(\mathcal{G})$ in $\mathcal{N}_\varepsilon(\mathcal{G})$. [In the case of a noncentrosymmetric normalizer, the index of \mathcal{G} in $\mathcal{N}_\varepsilon(\mathcal{G})$ is given as the product $k_g n_k$, where k_g means the index of \mathcal{G} in $\mathcal{K}(\mathcal{G})$ and n_k the index of $\mathcal{K}(\mathcal{G})$ in $\mathcal{N}_\varepsilon(\mathcal{G})$ or $\mathcal{N}_{\varepsilon^+}(\mathcal{G})$.] For continuous translations, k_g is always infinite. Nevertheless, it is useful to distinguish different cases: ∞, ∞^2 and ∞^3 refer to one, two and three independent directions with continuous translations. An additional factor of 2^n or 3^n indicates the existence of n additional independent translations which are not continuous.

For triclinic space groups, each metrical specialization gives rise to a symmetry enhancement of the Euclidean normalizer. The corresponding conditions for the metrical parameters, however, cannot be described as easily as in the monoclinic case (for further information see Chapter 3.1 and the literature on ‘reduced cells’ cited therein). Table 3.5.2.2 shows the Euclidean normalizers for $P1$ and $P\bar{1}$. Each special metrical condition is designated by the Bravais type of the corresponding translation lattice. In the case of $P\bar{1}$, the Euclidean normalizer is always the eigensymmetry group of a suitably chosen point lattice with basis vectors $\frac{1}{2}\mathbf{a}_c, \frac{1}{2}\mathbf{b}_c$ and $\frac{1}{2}\mathbf{c}_c$. Here, $\mathbf{a}_c, \mathbf{b}_c$ and \mathbf{c}_c do not refer to the primitive unit cell of $P\bar{1}$ but to the possibly centred conventional cell for the respective Bravais lattice. In the case of $P1$, the Euclidean normalizer always contains continuous translations in three independent directions, symbolized by P^3 . These normalizers may be easily derived from those for $P\bar{1}$.

3.5.2.2. Affine normalizers of plane groups and space groups

The affine normalizer $\mathcal{N}_A(\mathcal{G})$ of a space (plane) group \mathcal{G} either is a true supergroup of its Euclidean normalizer $\mathcal{N}_\varepsilon(\mathcal{G})$, or both normalizers coincide:

$$\mathcal{N}_A(\mathcal{G}) \geq \mathcal{N}_\varepsilon(\mathcal{G}).$$

As any translation is an isometry, each translation belonging to $\mathcal{N}_A(\mathcal{G})$ also belongs to $\mathcal{N}_\varepsilon(\mathcal{G})$. Therefore, the affine normalizer and the Euclidean normalizer of a space (plane) group necessarily have identical translation subgroups.

By analogy to the isometries of the Euclidean normalizer, the additional mappings of the affine normalizer also map the set of all symmetry elements of the space (plane) group onto itself.

In contrast to the Euclidean normalizers, the affine normalizers of all space (plane) groups of a certain type belong to only one type of normalizer, *i.e.* they are isomorphic groups. Therefore, the type of the affine normalizer $\mathcal{N}_A(\mathcal{G})$ never depends on the metrical properties of the space group \mathcal{G} .

If for all space (plane) groups of a certain type the Euclidean normalizers also belong to one type, then for each such space (plane) group the Euclidean and the affine normalizer are identical, irrespective of any metrical specialization, *i.e.* $\mathcal{N}_\varepsilon(\mathcal{G}) = \mathcal{N}_A(\mathcal{G})$ holds. Then, the affine normalizers are pure groups of motions and do not contain any further affine mappings. This is true for all cubic, hexagonal, trigonal and tetragonal space groups (for all hexagonal and square plane groups) and, in addition, for the space groups of 21 further orthorhombic types (plane groups of 4 further rectangular types) [examples: $\mathcal{N}_A(Pcca) = Pmmm$, $\mathcal{N}_A(Pnc2) = P^1mmm$].

² In previous editions, the symbols Z^1, Z^2 and Z^3 (z^1, z^2) were used.

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of \mathcal{G} in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$	
No.	Hermann-Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at		Further generators
5	C121	General	$P^1 12/m1$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$(2 \cdot \infty) \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 121$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$0, s, 0; 0, 0, \frac{1}{2}$	/		$(2 \cdot \infty) \cdot 1$
		$\beta = 90^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	\bar{x}, y, z	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 222$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$0, s, 0; 0, 0, \frac{1}{2}$	/	\bar{x}, y, \bar{z}	$(2 \cdot \infty) \cdot 2$
		$\cos \beta = -c/a, 90^\circ < \beta < 135^\circ$	$P^1 mmm$	$\frac{1}{2}(\mathbf{a} + \mathbf{c}), \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$x, y, 2x - z$	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 222$	$\frac{1}{2}(\mathbf{a} + \mathbf{c}), \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$0, s, 0; 0, 0, \frac{1}{2}$	/	$x, \bar{y}, 2x - z$	$(2 \cdot \infty) \cdot 2$
		$2 \cos \beta = -a/c, 90^\circ < \beta < 135^\circ$	$B^1 mmm$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{a} + \mathbf{c}$	$0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x} + z, y, z$	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): B^1 222$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{a} + \mathbf{c}$	$0, s, 0; 0, 0, \frac{1}{2}$	/	$\bar{x} + z, \bar{y}, z$	$(2 \cdot \infty) \cdot 2$
		$a = c\sqrt{2}, \beta = 135^\circ$	$P^1 4/mmm$	$-\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{c}, \mathbf{eb}$	$0, s, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	$x, y, 2x - z; \bar{x} + z, y, z$	$(2 \cdot \infty) \cdot 2 \cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 422$	$-\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{c}, \mathbf{eb}$	$0, s, 0; 0, 0, \frac{1}{2}$	/	$x, \bar{y}, 2x - z; \bar{x} + z, \bar{y}, z$	$(2 \cdot \infty) \cdot 4$
5	A121	General	$P^1 12/m1$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, s, 0$	$0, 0, 0$		$(2 \cdot \infty) \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 121$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, s, 0$	/		$(2 \cdot \infty) \cdot 1$
		$\beta = 90^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, s, 0$	$0, 0, 0$	\bar{x}, y, z	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 222$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, s, 0$	/	\bar{x}, y, \bar{z}	$(2 \cdot \infty) \cdot 2$
		$\cos \beta = -a/c, 90^\circ < \beta < 135^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}(\mathbf{a} + \mathbf{c})$	$\frac{1}{2}, 0, 0; 0, s, 0$	$0, 0, 0$	$\bar{x} + 2z, y, z$	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 222$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}(\mathbf{a} + \mathbf{c})$	$\frac{1}{2}, 0, 0; 0, s, 0$	/	$\bar{x} + 2z, \bar{y}, z$	$(2 \cdot \infty) \cdot 2$
		$2 \cos \beta = -c/a, 90^\circ < \beta < 135^\circ$	$B^1 mmm$	$\mathbf{a} + \frac{1}{2}\mathbf{c}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, s, 0$	$0, 0, 0$	$x, y, x - z$	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): B^1 222$	$\mathbf{a} + \frac{1}{2}\mathbf{c}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, s, 0$	/	$x, \bar{y}, x - z$	$(2 \cdot \infty) \cdot 2$
		$c = a\sqrt{2}, \beta = 135^\circ$	$P^1 4/mmm$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a} + \mathbf{c}), \mathbf{eb}$	$\frac{1}{2}, 0, 0; 0, s, 0$	$0, 0, 0$	$x, y, x - z; \bar{x} + 2z, y, z$	$(2 \cdot \infty) \cdot 2 \cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 422$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a} + \mathbf{c}), \mathbf{eb}$	$\frac{1}{2}, 0, 0; 0, s, 0$	/	$x, \bar{y}, x - z; \bar{x} + 2z, \bar{y}, z$	$(2 \cdot \infty) \cdot 4$
5	I121	General	$P^1 12/m1$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, s, 0$	$0, 0, 0$		$(2 \cdot \infty) \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 121$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, s, 0$	/		$(2 \cdot \infty) \cdot 1$
		$a > c, \beta = 90^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, s, 0$	$0, 0, 0$	\bar{x}, y, z	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 222$	$\frac{1}{2}\mathbf{a}, \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, s, 0$	/	\bar{x}, \bar{y}, z	$(2 \cdot \infty) \cdot 2$
		$\cos \beta = -c/a, 90^\circ < \beta < 180^\circ$	$P^1 mmm$	$\frac{1}{2}(\mathbf{a} + \mathbf{c}), \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, s, 0$	$0, 0, 0$	$x, y, 2x - z$	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 222$	$\frac{1}{2}(\mathbf{a} + \mathbf{c}), \mathbf{eb}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, s, 0$	/	$x, \bar{y}, 2x - z$	$(2 \cdot \infty) \cdot 2$
		$a = c, 90^\circ < \beta < 180^\circ$	$B^1 mmm$	$\frac{1}{2}(\mathbf{a} + \mathbf{c}), \mathbf{eb}, \frac{1}{2}(-\mathbf{a} + \mathbf{c})$	$\frac{1}{2}, 0, 0; 0, s, 0$	$0, 0, 0$	z, y, x	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): B^1 222$	$\frac{1}{2}(\mathbf{a} + \mathbf{c}), \mathbf{eb}, \frac{1}{2}(-\mathbf{a} + \mathbf{c})$	$\frac{1}{2}, 0, 0; 0, s, 0$	/	z, \bar{y}, x	$(2 \cdot \infty) \cdot 2$
		$a = c, \beta = 90^\circ$	$P^1 4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \mathbf{eb}$	$\frac{1}{2}, 0, 0; 0, s, 0$	$0, 0, 0$	$\bar{x}, y, z; z, y, x$	$(2 \cdot \infty) \cdot 2 \cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 422$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \mathbf{eb}$	$\frac{1}{2}, 0, 0; 0, s, 0$	/	$\bar{x}, \bar{y}, z; z, \bar{y}, x$	$(2 \cdot \infty) \cdot 4$
5	A112	General	$P^1 112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \mathbf{ec}$	$\frac{1}{2}, 0, 0; 0, 0, t$	$0, 0, 0$		$(2 \cdot \infty) \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 112$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \mathbf{ec}$	$\frac{1}{2}, 0, 0; 0, 0, t$	/		$(2 \cdot \infty) \cdot 1$
		$\gamma = 90^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \mathbf{ec}$	$\frac{1}{2}, 0, 0; 0, 0, t$	$0, 0, 0$	\bar{x}, y, z	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \mathbf{ec}$	$\frac{1}{2}, 0, 0; 0, 0, t$	/	\bar{x}, y, \bar{z}	$(2 \cdot \infty) \cdot 2$
		$\cos \gamma = -a/b, 90^\circ < \gamma < 135^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a} + \mathbf{b}), \mathbf{ec}$	$\frac{1}{2}, 0, 0; 0, 0, t$	$0, 0, 0$	$\bar{x} + 2y, y, z$	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a} + \mathbf{b}), \mathbf{ec}$	$\frac{1}{2}, 0, 0; 0, 0, t$	/	$\bar{x} + 2y, y, \bar{z}$	$(2 \cdot \infty) \cdot 2$
		$2 \cos \gamma = -b/a, 90^\circ < \gamma < 135^\circ$	$C^1 mmm$	$\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \mathbf{ec}$	$\frac{1}{2}, 0, 0; 0, 0, t$	$0, 0, 0$	$x, x - y, z$	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): C^1 222$	$\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \mathbf{ec}$	$\frac{1}{2}, 0, 0; 0, 0, t$	/	$x, x - y, \bar{z}$	$(2 \cdot \infty) \cdot 2$
		$b = a\sqrt{2}, \gamma = 135^\circ$	$P^1 4/mmm$	$-\frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{a}, \mathbf{ec}$	$\frac{1}{2}, 0, 0; 0, 0, t$	$0, 0, 0$	$\bar{x} + 2y, y, z; x, x - y, z$	$(2 \cdot \infty) \cdot 2 \cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 422$	$-\frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{a}, \mathbf{ec}$	$\frac{1}{2}, 0, 0; 0, 0, t$	/	$\bar{x} + 2y, y, \bar{z}; x, x - y, \bar{z}$	$(2 \cdot \infty) \cdot 4$
5	B112	General	$P^1 112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \mathbf{ec}$	$0, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$		$(2 \cdot \infty) \cdot 2 \cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 112$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \mathbf{ec}$	$0, \frac{1}{2}, 0; 0, 0, t$	/		$(2 \cdot \infty) \cdot 1$
		$\gamma = 90^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \mathbf{ec}$	$0, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	\bar{x}, y, z	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \mathbf{ec}$	$0, \frac{1}{2}, 0; 0, 0, t$	/	\bar{x}, y, \bar{z}	$(2 \cdot \infty) \cdot 2$
		$\cos \gamma = -b/a, 90^\circ < \gamma < 135^\circ$	$P^1 mmm$	$\frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{b}, \mathbf{ec}$	$0, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	$x, 2x - y, z$	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 222$	$\frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{b}, \mathbf{ec}$	$0, \frac{1}{2}, 0; 0, 0, t$	/	$x, 2x - y, \bar{z}$	$(2 \cdot \infty) \cdot 2$
		$2 \cos \gamma = -a/b, 90^\circ < \gamma < 135^\circ$	$C^1 mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a} + \mathbf{b}, \mathbf{ec}$	$0, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	$\bar{x} + y, y, z$	$(2 \cdot \infty) \cdot 2 \cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): C^1 222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a} + \mathbf{b}, \mathbf{ec}$	$0, \frac{1}{2}, 0; 0, 0, t$	/	$\bar{x} + y, y, \bar{z}$	$(2 \cdot \infty) \cdot 2$
		$a = b\sqrt{2}, \gamma = 135^\circ$	$P^1 4/mmm$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a} + \mathbf{b}), \mathbf{ec}$	$0, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	$x, 2x - y, z; \bar{x} + y, y, z$	$(2 \cdot \infty) \cdot 2 \cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1 422$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a} + \mathbf{b}), \mathbf{ec}$	$0, \frac{1}{2}, 0; 0, 0, t$	/	$x, 2x - y, \bar{z}; \bar{x} + y, y, \bar{z}$	$(2 \cdot \infty) \cdot 4$

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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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of \mathcal{G} in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$	
No.	Hermann– Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at		Further generators
8	<i>C1m1</i>	General	$P^212/m1$	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	$\infty^2 \cdot 2 \cdot 1$	
		$\beta = 90^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 2$
		$\cos \beta = -c/a, 90^\circ < \beta < 135^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a} + \mathbf{c}), \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	$x, y, 2x - z$	$\infty^2 \cdot 2 \cdot 2$
		$2 \cos \beta = -a/c, 90^\circ < \beta < 135^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2(\frac{1}{2} \mathbf{a} + \mathbf{c})$	$r, 0, 0; 0, 0, t$	0, 0, 0	$\bar{x} + z, y, z$	$\infty^2 \cdot 2 \cdot 2$
8	<i>A1m1</i>	$a = c\sqrt{2}, \beta = 135^\circ$	P^24/mmm	$-\varepsilon(\mathbf{a} + \mathbf{c}), \varepsilon \mathbf{c}, \frac{1}{2} \mathbf{b}$	$r, 0, 0; 0, 0, t$	0, 0, 0	$x, y, 2x - z; \bar{x} + z, y, z$	$\infty^2 \cdot 2 \cdot 4$
		General	$P^212/m1$	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 1$
		$\beta = 90^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 2$
		$\cos \beta = -a/c, 90^\circ < \beta < 135^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2(\mathbf{a} + \mathbf{c})$	$r, 0, 0; 0, 0, t$	0, 0, 0	$\bar{x} + 2z, y, z$	$\infty^2 \cdot 2 \cdot 2$
8	<i>I1m1</i>	$2 \cos \beta = -c/a, 90^\circ < \beta < 135^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a} + \frac{1}{2} \mathbf{c}), \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	$x, y, x - z$	$\infty^2 \cdot 2 \cdot 2$
		$c = a\sqrt{2}, \beta = 135^\circ$	P^24/mmm	$\varepsilon \mathbf{a}, -\varepsilon(\mathbf{a} + \mathbf{c}), \frac{1}{2} \mathbf{b}$	$r, 0, 0; 0, 0, t$	0, 0, 0	$x, y, x - z; \bar{x} + 2z, y, z$	$\infty^2 \cdot 2 \cdot 4$
		General	$P^212/m1$	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 1$
		$a > c, \beta = 90^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 2$
8	<i>A11m</i>	$\cos \beta = -c/a, 90^\circ < \beta < 180^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a} + \mathbf{c}), \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	$x, y, 2x - z$	$\infty^2 \cdot 2 \cdot 2$
		$a = c, 90^\circ < \beta < 180^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a} + \mathbf{c}), \frac{1}{2} \mathbf{b}, \varepsilon_2(-\mathbf{a} + \mathbf{c})$	$r, 0, 0; 0, 0, t$	0, 0, 0	z, y, x	$\infty^2 \cdot 2 \cdot 2$
		$a = c, \beta = 90^\circ$	P^24/mmm	$\varepsilon \mathbf{c}, \varepsilon \mathbf{a}, \frac{1}{2} \mathbf{b}$	$r, 0, 0; 0, 0, t$	0, 0, 0	$\bar{x}, y, z; z, y, x$	$\infty^2 \cdot 2 \cdot 4$
		General	P^2112/m	$\varepsilon_1 \mathbf{a}, \varepsilon_2 \mathbf{b}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 1$
8	<i>B11m</i>	$\gamma = 90^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \varepsilon_2 \mathbf{b}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 2$
		$\cos \gamma = -a/b, 90^\circ < \gamma < 135^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \varepsilon_2(\mathbf{a} + \mathbf{b}), \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	$\bar{x} + 2y, y, z$	$\infty^2 \cdot 2 \cdot 2$
		$2 \cos \gamma = -b/a, 90^\circ < \gamma < 135^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a} + \frac{1}{2} \mathbf{b}), \varepsilon_2 \mathbf{b}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	$x, x - y, z$	$\infty^2 \cdot 2 \cdot 2$
		$b = a\sqrt{2}, \gamma = 135^\circ$	P^24/mmm	$-\varepsilon(\mathbf{a} + \mathbf{b}), \varepsilon \mathbf{a}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	$\bar{x} + 2y, y, z; x, x - y, z$	$\infty^2 \cdot 2 \cdot 4$
8	<i>I11m</i>	General	P^2112/m	$\varepsilon_1 \mathbf{a}, \varepsilon_2 \mathbf{b}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 1$
		$\gamma = 90^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \varepsilon_2 \mathbf{b}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 2$
		$\cos \gamma = -b/a, 90^\circ < \gamma < 180^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a} + \mathbf{b}), \varepsilon_2 \mathbf{b}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	$x, 2x - y, z$	$\infty^2 \cdot 2 \cdot 2$
		$2 \cos \gamma = -a/b, 90^\circ < \gamma < 180^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \varepsilon_2(\frac{1}{2} \mathbf{a} + \mathbf{b}), \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	$\bar{x} + y, y, z$	$\infty^2 \cdot 2 \cdot 2$
8	<i>I11m</i>	$a = b\sqrt{2}, \gamma = 135^\circ$	P^24/mmm	$\varepsilon \mathbf{b}, -\varepsilon(\mathbf{a} + \mathbf{b}), \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	$x, 2x - y, z; \bar{x} + y, y, z$	$\infty^2 \cdot 2 \cdot 4$
		General	P^2112/m	$\varepsilon_1 \mathbf{a}, \varepsilon_2 \mathbf{b}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 1$
		$a < b, \gamma = 90^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \varepsilon_2 \mathbf{b}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 2$
		$\cos \gamma = -a/b, 90^\circ < \gamma < 180^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \varepsilon_2(\mathbf{a} + \mathbf{b}), \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	$\bar{x} + 2y, y, z$	$\infty^2 \cdot 2 \cdot 2$
9	<i>C1c1</i>	$a = b, 90^\circ < \gamma < 180^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a} - \mathbf{b}), \varepsilon_2(\mathbf{a} + \mathbf{b}), \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	y, x, z	$\infty^2 \cdot 2 \cdot 2$
		$a = b, \gamma = 90^\circ$	P^24/mmm	$\varepsilon \mathbf{a}, \varepsilon \mathbf{b}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	$\bar{x}, y, z; y, x, z$	$\infty^2 \cdot 2 \cdot 4$
		General	$P^212/m1$	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 1$
		$\beta = 90^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 2$
9	<i>A1n1</i>	$\cos \beta = -c/a, 90^\circ < \beta < 135^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a} + \mathbf{c}), \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	$x, y, 2x - z$	$\infty^2 \cdot 2 \cdot 2$
		$2 \cos \beta = -a/c, 90^\circ < \beta < 135^\circ$	P^2bmb	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2(\frac{1}{2} \mathbf{a} + \mathbf{c})$	$r, 0, 0; 0, 0, t$	0, 0, 0	$\bar{x} + z, y + \frac{1}{4}, z$	$\infty^2 \cdot 2 \cdot 2$
		$a = c\sqrt{2}, \beta = 135^\circ$	P^24_2/mmc	$-\varepsilon(\mathbf{a} + \mathbf{c}), \varepsilon \mathbf{c}, \frac{1}{2} \mathbf{b}$	$r, 0, 0; 0, 0, t$	0, 0, 0	$x, y, 2x - z; \bar{x} + z, y + \frac{1}{4}, z$	$\infty^2 \cdot 2 \cdot 4$
		General	$P^212/m1$	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 1$
9	<i>I1a1</i>	$\beta = 90^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 2$
		$\cos \beta = -a/c, 90^\circ < \beta < 135^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \frac{1}{2} \mathbf{b}, \varepsilon_2(\mathbf{a} + \mathbf{c})$	$r, 0, 0; 0, 0, t$	0, 0, 0	$\bar{x} + 2z, y, z$	$\infty^2 \cdot 2 \cdot 2$
		$2 \cos \beta = -c/a, 90^\circ < \beta < 135^\circ$	P^2bmb	$\varepsilon_1(\mathbf{a} + \frac{1}{2} \mathbf{c}), \frac{1}{2} \mathbf{b}, \varepsilon_2 \mathbf{c}$	$r, 0, 0; 0, 0, t$	0, 0, 0	$x, y + \frac{1}{4}, x - z$	$\infty^2 \cdot 2 \cdot 2$
		$c = a\sqrt{2}, \beta = 135^\circ$	P^24_2/mmc	$\varepsilon \mathbf{a}, -\varepsilon(\mathbf{a} + \mathbf{c}), \frac{1}{2} \mathbf{b}$	$r, 0, 0; 0, 0, t$	0, 0, 0	$x, y + \frac{1}{4}, x - z; \bar{x} + 2z, y, z$	$\infty^2 \cdot 2 \cdot 4$
9	<i>A11a</i>	General	P^2112/m	$\varepsilon_1 \mathbf{a}, \varepsilon_2 \mathbf{b}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 1$
		$\gamma = 90^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \varepsilon_2 \mathbf{b}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 2$
		$\cos \gamma = -a/b, 90^\circ < \gamma < 135^\circ$	P^2mmm	$\varepsilon_1 \mathbf{a}, \varepsilon_2(\mathbf{a} + \mathbf{b}), \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	$\bar{x} + 2y, y, z$	$\infty^2 \cdot 2 \cdot 2$
		$2 \cos \gamma = -b/a, 90^\circ < \gamma < 135^\circ$	P^2ccm	$\varepsilon_1(\mathbf{a} + \frac{1}{2} \mathbf{b}), \varepsilon_2 \mathbf{b}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	$x, x - y, z + \frac{1}{4}$	$\infty^2 \cdot 2 \cdot 2$
9	<i>A11a</i>	$b = a\sqrt{2}, \gamma = 135^\circ$	P^24_2/mmc	$-\varepsilon(\mathbf{a} + \mathbf{b}), \varepsilon \mathbf{a}, \frac{1}{2} \mathbf{c}$	$r, 0, 0; 0, s, 0$	0, 0, 0	$\bar{x} + 2y, y, z; x, x - y, z + \frac{1}{4}$	$\infty^2 \cdot 2 \cdot 4$

3.5. NORMALIZERS OF SPACE GROUPS

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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of \mathcal{G} in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$	
No.	Hermann-Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at		Further generators
9	$B11n$	General	P^2112/m	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0$	$0, 0, 0$	$\infty^2 \cdot 2 \cdot 1$	
		$\gamma=90^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0$	$0, 0, 0$	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 2$
		$\cos \gamma = -b/a, 90^\circ < \gamma < 135^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{b}), \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0$	$0, 0, 0$	$x, 2x-y, z$	$\infty^2 \cdot 2 \cdot 2$
		$2 \cos \gamma = -a/b, 90^\circ < \gamma < 135^\circ$	P^2ccm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0$	$0, 0, 0$	$\bar{x}+y, y, z+\frac{1}{4}$	$\infty^2 \cdot 2 \cdot 2$
9	$I11b$	General	P^2112/m	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0$	$0, 0, 0$	$\infty^2 \cdot 2 \cdot 1$	
		$a < b, \gamma = 90^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0$	$0, 0, 0$	\bar{x}, y, z	$\infty^2 \cdot 2 \cdot 2$
		$\cos \gamma = -a/b, 90^\circ < \gamma < 180^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0$	$0, 0, 0$	$\bar{x}+2y, y, z$	$\infty^2 \cdot 2 \cdot 2$
		$a = b, 90^\circ < \gamma < 180^\circ$	P^2ccm	$\varepsilon_1(\mathbf{a}-\mathbf{b}), \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0; 0, s, 0$	$0, 0, 0$	$y, x, z+\frac{1}{4}$	$\infty^2 \cdot 2 \cdot 2$
10	$P12/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$8 \cdot 1 \cdot 1$	
		$a > c, \beta = 90^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		\bar{x}, y, z	$8 \cdot 1 \cdot 2$
		$2 \cos \beta = -c/a, 90^\circ < \beta < 120^\circ$	$Bmnm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, y, x-z$	$8 \cdot 1 \cdot 2$
		$a = c, 90^\circ < \beta < 120^\circ$	$Bmnm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		z, y, x	$8 \cdot 1 \cdot 2$
10	$P112/m$	General	$P4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$8 \cdot 1 \cdot 4$	
		$a = c, \beta = 120^\circ$	$P6/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z; z, y, x$	$8 \cdot 1 \cdot 6$
		$a < b, \gamma = 90^\circ$	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$z, y, x; \bar{x}+z, y, z$	$8 \cdot 1 \cdot 6$
		$2 \cos \gamma = -a/b, 90^\circ < \gamma < 120^\circ$	$Pnmn$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		\bar{x}, y, z	$8 \cdot 1 \cdot 2$
11	$P12_1/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$8 \cdot 1 \cdot 1$	
		$a > c, \beta = 90^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		\bar{x}, y, z	$8 \cdot 1 \cdot 2$
		$2 \cos \beta = -c/a, 90^\circ < \beta < 120^\circ$	$Bmnm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, y, x-z$	$8 \cdot 1 \cdot 2$
		$a = c, 90^\circ < \beta < 120^\circ$	$Bmnm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		z, y, x	$8 \cdot 1 \cdot 2$
11	$P112_1/m$	General	$P4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$8 \cdot 1 \cdot 4$	
		$a = c, \beta = 120^\circ$	$P6/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z; z, y, x$	$8 \cdot 1 \cdot 6$
		$a < b, \gamma = 90^\circ$	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$z, y, x; \bar{x}+z, y, z$	$8 \cdot 1 \cdot 6$
		$2 \cos \gamma = -a/b, 90^\circ < \gamma < 120^\circ$	$Pnmn$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		\bar{x}, y, z	$8 \cdot 1 \cdot 2$
12	$C12/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		$4 \cdot 1 \cdot 1$	
		$\beta = 90^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		\bar{x}, y, z	$4 \cdot 1 \cdot 2$
		$\cos \beta = -c/a, 90^\circ < \beta < 135^\circ$	$Pmnm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		$x, y, 2x-z$	$4 \cdot 1 \cdot 2$
		$2 \cos \beta = -a/c, 90^\circ < \beta < 135^\circ$	$Bmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a}+\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		$\bar{x}+z, y, z$	$4 \cdot 1 \cdot 2$
12	$A12/m1$	General	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		$4 \cdot 1 \cdot 4$	
		$a = c\sqrt{2}, \beta = 135^\circ$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		$x, y, 2x-z; \bar{x}+z, y, z$	$4 \cdot 1 \cdot 4$
		$a > c, \beta = 90^\circ$	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		\bar{x}, y, z	$4 \cdot 1 \cdot 1$
		$\beta = 90^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		\bar{x}, y, z	$4 \cdot 1 \cdot 2$
12	$I12/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$4 \cdot 1 \cdot 1$	
		$a > c, \beta = 90^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		\bar{x}, y, z	$4 \cdot 1 \cdot 2$
		$\cos \beta = -c/a, 90^\circ < \beta < 180^\circ$	$Pmnm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$x, y, 2x-z$	$4 \cdot 1 \cdot 2$
		$a = c, 90^\circ < \beta < 180^\circ$	$Bmnm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		z, y, x	$4 \cdot 1 \cdot 2$
12	$I12/m1$	General	$P4/mmm$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$4 \cdot 1 \cdot 4$	
		$c = a\sqrt{2}, \beta = 135^\circ$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$x, y, x-z; \bar{x}+2z, y, z$	$4 \cdot 1 \cdot 4$
		$a > c, \beta = 90^\circ$	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		\bar{x}, y, z	$4 \cdot 1 \cdot 1$
		$\beta = 90^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		\bar{x}, y, z	$4 \cdot 1 \cdot 2$

3.5. NORMALIZERS OF SPACE GROUPS

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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Index of \mathcal{G} in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		
No.	Hermann-Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations		Inversion through a centre at Further generators	
14	$P12_1/n1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		8-1-1	
		$a > c, \beta = 90^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		\bar{x}, y, z	8-1-2
		$\cos \beta = -c/a, 90^\circ < \beta < 180^\circ$	$Pmnm$	$\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, y, 2x - z$	8-1-2
		$a = c, 90^\circ < \beta < 180^\circ$	$Bmnm$	$\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a} + \mathbf{c})$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		z, y, x	8-1-2
14	$P12_1/a1$	General	$P4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		8-1-4	
		$a = c, \beta = 90^\circ$	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z; z, y, x$	8-1-4
		$\beta = 90^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		\bar{x}, y, z	8-1-2
		$\cos \beta = -c/a, 90^\circ < \beta < 135^\circ$	$Pmnm$	$\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, y, 2x - z$	8-1-2
14	$P112_1/a$	General	$Bmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		8-1-2	
		$2 \cos \beta = -a/c, 90^\circ < \beta < 135^\circ$	$Bmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x} + z, y, z$	8-1-2
		$a = c\sqrt{2}, \beta = 135^\circ$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, y, 2x - z; \bar{x} + z, y, z$	8-1-4
		$a = c\sqrt{2}, \beta = 135^\circ$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, y, 2x - z; \bar{x} + z, y, z$	8-1-4
14	$P112_1/n$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		8-1-1	
		$a < b, \gamma = 90^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		\bar{x}, y, z	8-1-2
		$\cos \gamma = -a/b, 90^\circ < \gamma < 180^\circ$	$Pmnm$	$\frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, 2x - y, z$	8-1-2
		$2 \cos \gamma = -a/b, 90^\circ < \gamma < 135^\circ$	$Cmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a} + \mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x} + y, y, z$	8-1-2
14	$P112_1/b$	General	$P4/mmm$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		8-1-4	
		$a = b, \gamma = 90^\circ$	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, 2x - y, z; \bar{x} + y, y, z$	8-1-4
		$a < b, \gamma = 90^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		\bar{x}, y, z	8-1-2
		$\cos \gamma = -a/b, 90^\circ < \gamma < 180^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x} + 2y, y, z$	8-1-2
14	$P112_1/b$	General	$Cmmm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		8-1-2	
		$2 \cos \gamma = -b/a, 90^\circ < \gamma < 135^\circ$	$Cmmm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		y, x, z	8-1-2
		$a = b, \gamma = 90^\circ$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x}, y, z; y, x, z$	8-1-4
		$a = b, \gamma = 90^\circ$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		\bar{x}, y, z	8-1-2
15	$C12/c1$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		8-1-1	
		$\beta = 90^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		\bar{x}, y, z	4-1-2
		$\cos \beta = -c/a, 90^\circ < \beta < 135^\circ$	$Pmnm$	$\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$x, y, 2x - z$	4-1-2
		$2 \cos \beta = -a/c, 90^\circ < \beta < 135^\circ$	$Bbmb$ ($n2/mn$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		$\bar{x} + z + \frac{1}{4}, y + \frac{1}{4}, z$	4-1-2
15	$A12/n1$	General	$P4_2/mmc$ ($2/m2/mn$)	$-\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		4-1-4	
		$a = c\sqrt{2}, \beta = 135^\circ$	$P4_2/mmc$ ($2/m2/mn$)	$-\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		$x, y, 2x - z; \bar{x} + z + \frac{1}{4}, y + \frac{1}{4}, z$	4-1-4
		$\beta = 90^\circ$	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		\bar{x}, y, z	4-1-1
		$\cos \beta = -a/c, 90^\circ < \beta < 135^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$\bar{x} + 2z, y, z$	4-1-2
15	$I12/a1$	General	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}(\mathbf{a} + \mathbf{c}),$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		4-1-2	
		$2 \cos \beta = -c/a, 90^\circ < \beta < 135^\circ$	$Bbmb$ ($n2/mn$)	$\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$x, y + \frac{1}{4}, x - z + \frac{1}{4}$	4-1-2
		$c = a\sqrt{2}, \beta = 135^\circ$	$P4_2/mmc$ ($2/m2/mn$)	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$\bar{x} + 2z, y, z; x, y + \frac{1}{4}, x - z + \frac{1}{4}$	4-1-4
		$c = a\sqrt{2}, \beta = 135^\circ$	$P4_2/mmc$ ($2/m2/mn$)	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$\bar{x} + 2z, y, z; x, y + \frac{1}{4}, x - z + \frac{1}{4}$	4-1-4
15	$A112/a$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		4-1-1	
		$a > c, \beta = 90^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		\bar{x}, y, z	4-1-2
		$\cos \beta = -c/a, 90^\circ < \beta < 180^\circ$	$Pmnm$	$\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$x, y, 2x - z$	4-1-2
		$a = c, 90^\circ < \beta < 180^\circ$	$Bbmb$ ($n2/mn$)	$\frac{1}{2}(\mathbf{a} + \mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a} + \mathbf{c})$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$z + \frac{1}{4}, y + \frac{1}{4}, x + \frac{1}{4}$	4-1-2
15	$A112/a$	General	$P4_2/mmc$ ($2/m2/mn$)	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		4-1-4	
		$a = c, \beta = 90^\circ$	$P4_2/mmc$ ($2/m2/mn$)	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$\bar{x}, y, z; z + \frac{1}{4}, y + \frac{1}{4}, x + \frac{1}{4}$	4-1-4
		$\beta = 90^\circ$	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		\bar{x}, y, z	4-1-1
		$\cos \gamma = -a/b, 90^\circ < \gamma < 135^\circ$	$Pmnm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$\bar{x} + 2y, y, z$	4-1-2
15	$A112/a$	General	$Cccm$ ($n n2/m$)	$\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		4-1-2	
		$2 \cos \gamma = -b/a, 90^\circ < \gamma < 135^\circ$	$Cccm$ ($n n2/m$)	$\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$x, x - y + \frac{1}{4}, z + \frac{1}{4}$	4-1-2
		$b = a\sqrt{2}, \gamma = 135^\circ$	$P4_2/mmc$ ($2/m2/mn$)	$-\frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$\bar{x} + 2y, y, z;$ $x, x - y + \frac{1}{4}, z + \frac{1}{4}$	4-1-4
		$b = a\sqrt{2}, \gamma = 135^\circ$	$P4_2/mmc$ ($2/m2/mn$)	$-\frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$\bar{x} + 2y, y, z;$ $x, x - y + \frac{1}{4}, z + \frac{1}{4}$	4-1-4

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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of \mathcal{G} in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$	
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at		Further generators
15	$B112/n$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$			4.1.1
		$\gamma=90^\circ$	$Pm\bar{m}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		x, \bar{y}, z	4.1.2
		$\cos \gamma = -b/a, 90^\circ < \gamma < 135^\circ$	$Pm\bar{m}m$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$x, 2x-y, z$	4.1.2
		$2 \cos \gamma = -a/b, 90^\circ < \gamma < 135^\circ$	$Cccm$ ($n n 2/m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$\bar{x}+y+\frac{1}{4}, y, z+\frac{1}{4}$	4.1.2
		$a=b\sqrt{2}, \gamma=135^\circ$	$P4_2/mmc$ ($2/m2/mn$)	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$x, 2x-y, z;$ $\bar{x}+y+\frac{1}{4}, y, z+\frac{1}{4}$	4.1.4
15	$I112/b$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$			4.1.1
		$a < b, \gamma = 90^\circ$	$Pm\bar{m}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		\bar{x}, y, z	4.1.2
		$\cos \gamma = -a/b, 90^\circ < \gamma < 180^\circ$	$Pm\bar{m}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$\bar{x}+2y, y, z$	4.1.2
		$a = b, 90^\circ < \gamma < 180^\circ$	$Cccm$ ($n n 2/m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	4.1.2
		$a = b, \gamma = 90^\circ$	$P4_2/mmc$ ($2/m2/mn$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$\bar{x}, y, z; y+\frac{1}{4}, x+\frac{1}{4},$ $z+\frac{1}{4}$	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

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

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.

3.5. NORMALIZERS OF SPACE GROUPS

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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of \mathcal{G} in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
61	<i>Pbca</i>	$a \neq b$ or $b \neq c$ or $a \neq c$ $a = b = c$	<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
			<i>Pm</i> $\bar{3}$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$		z, x, y	$8 \cdot 1 \cdot 3$
62	<i>Pnma</i>		<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$8 \cdot 1 \cdot 1$
63	<i>Cmcm</i>		<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
64	<i>Cmce</i>		<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
65	<i>Cmmm</i>	$a \neq b$ $a = b$	<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
			<i>P4/mmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		y, x, z	$4 \cdot 1 \cdot 2$
66	<i>Cccm</i>	$a \neq b$ $a = b$	<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
			<i>P4/mmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		y, x, z	$4 \cdot 1 \cdot 2$
67	<i>Cmme</i>	$a \neq b$ $a = b$	<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
			<i>P4/mmm (mmm)</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		$y + \frac{1}{4}, x - \frac{1}{4}, z$	$4 \cdot 1 \cdot 2$
68	<i>Ccce (222)</i>	$a \neq b$ $a = b$	<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
			<i>P4/mmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		y, x, z	$4 \cdot 1 \cdot 2$
68	<i>Ccce ($\bar{1}$)</i>	$a \neq b$ $a = b$	<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
			<i>P4/mmm (mmm)</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}$		$y + \frac{1}{4}, x - \frac{1}{4}, z$	$4 \cdot 1 \cdot 2$
69	<i>Fmmm</i>	$a \neq b \neq c \neq a$ $a = b \neq c$ $a = b = c$	<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$			$2 \cdot 1 \cdot 1$
			<i>P4/mmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$		y, x, z	$2 \cdot 1 \cdot 2$
			<i>Pm</i> $\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$		$z, x, y; y, x, z$	$2 \cdot 1 \cdot 6$
70	<i>Fddd (222)</i>	$a \neq b \neq c \neq a$ $a = b \neq c$ $a = b = c$	<i>Pnnn (222)</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$			$2 \cdot 1 \cdot 1$
			<i>P4₂/nnm ($\bar{4}2m$)</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$		\bar{y}, \bar{x}, z	$2 \cdot 1 \cdot 2$
			<i>Pn</i> $\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$		$z, x, y; y, x, z$	$2 \cdot 1 \cdot 6$
70	<i>Fddd ($\bar{1}$)</i>	$a \neq b \neq c \neq a$ $a = b \neq c$ $a = b = c$	<i>Pnnn ($\bar{1}$)</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$			$2 \cdot 1 \cdot 1$
			<i>P4₂/nnm (2/m at $0, \frac{1}{2}, 0$)</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$		y, x, z	$2 \cdot 1 \cdot 2$
			<i>Pn</i> $\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0$		$z, x, y; y, x, z$	$2 \cdot 1 \cdot 6$
71	<i>Immm</i>	$a \neq b \neq c \neq a$ $a = b \neq c$ $a = b = c$	<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$			$4 \cdot 1 \cdot 1$
			<i>P4/mmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		y, x, z	$4 \cdot 1 \cdot 2$
			<i>Pm</i> $\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$z, x, y; y, x, z$	$4 \cdot 1 \cdot 6$
72	<i>Ibam</i>	$a \neq b$ $a = b$	<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$			$4 \cdot 1 \cdot 1$
			<i>P4/mmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		y, x, z	$4 \cdot 1 \cdot 2$
73	<i>Ibca</i>	$a \neq b \neq c \neq a$ $a = b \neq c$ $a = b = c$	<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$			$4 \cdot 1 \cdot 1$
			<i>P4₂/nmc (2/m 2/m n)</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$	$4 \cdot 1 \cdot 2$
			<i>Pm</i> $\bar{3}n$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$z, x, y; y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$	$4 \cdot 1 \cdot 6$
74	<i>Imma</i>	$a \neq b$ $a = b$	<i>Pmmm</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$			$4 \cdot 1 \cdot 1$
			<i>P4₂/nmc (2/m 2/m n)</i>	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$		$y + \frac{1}{4}, x - \frac{1}{4}, z + \frac{1}{4}$	$4 \cdot 1 \cdot 2$

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)

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	y, x, z	$(2 \cdot \infty) \cdot 2 \cdot 2$
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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, t$	$0, 0, 0$	y, x, z	$(2 \cdot \infty) \cdot 2 \cdot 2$
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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$	y, x, z	$\infty \cdot 2 \cdot 2$
80	$I4_1$	$P^14/nbm (\bar{4}2m)$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1422 (222)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$\frac{1}{4}, 0, 0$	y, x, \bar{z}	$\infty \cdot 2 \cdot 2$
81	$\bar{P}4$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	y, x, z	$4 \cdot 2 \cdot 2$
82	$\bar{I}4$	$I4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, \frac{1}{4}$	$0, 0, 0$	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	$I4_1/a (\bar{4})$	$P4_2/nmm (\bar{4}2m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		y, x, \bar{z}	$2 \cdot 1 \cdot 2$
88	$I4_1/a (\bar{1})$	$P4_2/nmm (2/m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		$y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$	$2 \cdot 1 \cdot 2$
89	$P422$	$P4/mmm$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4 \cdot 2 \cdot 1$
90	$P4_22$	$P4/mmm$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4 \cdot 1$
91	$P4_122$	$P4_222 (222 \text{ at } 4_212) [\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})]$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	/		$4 \cdot 2 \cdot 1$
92	$P4_212$	$P4_222 [\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})]$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	/		$4 \cdot 1$
93	$P4_222$	$P4/mmm$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4 \cdot 1$
94	$P4_22_12$	$P4/mmm$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4 \cdot 2 \cdot 1$
95	$P4_322$	$P4_222 (222 \text{ at } 4_212) [\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})]$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	/		$4 \cdot 1$
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	$I422$	$P4/mmm$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$0, 0, 0$		$2 \cdot 2 \cdot 1$
98	$I4_122$	$P4_2/nmm (\bar{4}2m)$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P4_222$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$\frac{1}{4}, 0, \frac{1}{8}$		$2 \cdot 1$
98			$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	/		$2 \cdot 2 \cdot 1$
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	$I4,md$	$P^14/nbm (\bar{4}2m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$\frac{1}{4}, 0, 0$		$\infty \cdot 2 \cdot 1$
110	$I4_c d$	$P^14/nbm (\bar{4}2m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, 0, t$	$\frac{1}{4}, 0, 0$		$\infty \cdot 2 \cdot 1$
111	$\bar{P}4_2m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4 \cdot 2 \cdot 1$
112	$\bar{P}4_2c$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4 \cdot 2 \cdot 1$
113	$\bar{P}4_2_1m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$		$4 \cdot 2 \cdot 1$

3.5. NORMALIZERS OF SPACE GROUPS

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	$P4_2c$	$P4/mmm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	0, 0, 0		$4 \cdot 2 \cdot 1$
115	$P4m2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	0, 0, 0		$4 \cdot 2 \cdot 1$
116	$P4c2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	0, 0, 0		$4 \cdot 2 \cdot 1$
117	$P4b2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	0, 0, 0		$4 \cdot 2 \cdot 1$
118	$P4n2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$	0, 0, 0		$4 \cdot 2 \cdot 1$
119	$I4m2$	$I4/mmm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, \frac{1}{4}$	0, 0, 0		$4 \cdot 2 \cdot 1$
120	$I4c2$	$I4/mmm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, \frac{1}{4}$	0, 0, 0		$4 \cdot 2 \cdot 1$
121	$I42m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	0, 0, $\frac{1}{2}$	0, 0, 0		$2 \cdot 2 \cdot 1$
122	$I42d$	$P4_2/nm (\bar{4}2m)$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	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	$P4/nmm (2/m)$	$P4/mmm (mnm)$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
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	$P4_2/nmm (\bar{4}2m)$	$P4/mmm$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
134	$P4_2/nmm (2/m)$	$P4/mmm (mmm)$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
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	$P4_2/nmc (\bar{1})$	$P4/mmm (mnm)$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, 0; 0, 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
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	$I4_1/amd (\bar{4}m2)$	$P4_2/nmm (\bar{4}2m)$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	0, 0, $\frac{1}{2}$			$2 \cdot 1 \cdot 1$
141	$I4_1/amd (2/m)$	$P4_2/nmm (2/m)$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	0, 0, $\frac{1}{2}$			$2 \cdot 1 \cdot 1$
142	$I4_1/acd (\bar{4})$	$P4_2/nmm (\bar{4}2m)$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	0, 0, $\frac{1}{2}$			$2 \cdot 1 \cdot 1$
142	$I4_1/acd (\bar{1})$	$P4_2/nmm (2/m)$	$\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \frac{1}{2}\mathbf{c}$	0, 0, $\frac{1}{2}$			$2 \cdot 1 \cdot 1$
143	$P3$	P^16/mmm $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1622$	$\frac{2}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, \mathbf{e}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, t$	0, 0, 0	$\bar{x}, \bar{y}, z; y, x, z$	$(3 \cdot \infty) \cdot 2 \cdot 4$
144	$P3_1$	$P^1622 [\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})]$	$\frac{2}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, \mathbf{e}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, t$	/	$\bar{x}, \bar{y}, z; y, x, \bar{z}$	$(3 \cdot \infty) \cdot 4$
145	$P3_2$	$P^1622 [\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})]$	$\frac{2}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, \mathbf{e}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, t$	/	$\bar{x}, \bar{y}, z; y, x, \bar{z}$	$(3 \cdot \infty) \cdot 4$
146	$R3$ (hexag.)	$P^1\bar{3}1m$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1312$	$\frac{2}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, \mathbf{e}\mathbf{c}$	0, 0, t	0, 0, 0	\bar{y}, \bar{x}, z	$\infty \cdot 2 \cdot 2$
146	$R3$ (rhomboh.)	$P^1\bar{3}1m$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1312$	$\frac{2}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, \mathbf{e}\mathbf{c}$ $\frac{2}{3}\mathbf{a} - \frac{1}{3}\mathbf{b} - \frac{1}{3}\mathbf{c}, -\frac{1}{3}\mathbf{a} + \frac{2}{3}\mathbf{b} - \frac{1}{3}\mathbf{c},$ $\varepsilon(\mathbf{a} + \mathbf{b} + \mathbf{c})$ $\frac{2}{3}\mathbf{a} - \frac{1}{3}\mathbf{b} - \frac{1}{3}\mathbf{c}, -\frac{1}{3}\mathbf{a} + \frac{2}{3}\mathbf{b} - \frac{1}{3}\mathbf{c},$ $\varepsilon(\mathbf{a} + \mathbf{b} + \mathbf{c})$	0, 0, t r, r, r r, r, r	/ 0, 0, 0	y, x, \bar{z} y, x, z $\bar{y}, \bar{x}, \bar{z}$	$\infty \cdot 2$ $\infty \cdot 2 \cdot 2$ $\infty \cdot 2$
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	$2 \cdot 1 \cdot 2$

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

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	$P312$	$P6/mmm$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P622$	$\frac{2}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, \frac{1}{2}\mathbf{c}$ $\frac{2}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, \frac{1}{2}$ $\frac{2}{3}, \frac{1}{3}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$ /	\bar{x}, \bar{y}, z \bar{x}, \bar{y}, z	$6 \cdot 2 \cdot 2$ $6 \cdot 2$
150	$P321$	$P6/mmm$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P622$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$ $\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$ $0, 0, \frac{1}{2}$	$0, 0, 0$ /	\bar{x}, \bar{y}, z \bar{x}, \bar{y}, z	$2 \cdot 2 \cdot 2$ $2 \cdot 2$
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	$R32$ (hexag.)	$R\bar{3}m$ (hexag.) $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): R32$ (hexag.)	$-\mathbf{a}, -\mathbf{b}, \frac{1}{2}\mathbf{c}$ $-\mathbf{a}, -\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$ $0, 0, \frac{1}{2}$	$0, 0, 0$ /		$2 \cdot 2 \cdot 1$ $2 \cdot 1$
155	$R32$ (rhomboh.)	$R\bar{3}m$ (rhomboh.) $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): R32$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c}), \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c}),$ $\frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c})$ $\frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c}), \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c}),$ $\frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c})$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, 0$ /		$2 \cdot 2 \cdot 1$ $2 \cdot 1$
156	$P3m1$	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	$P31m$	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	$P3c1$	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	$P31c$	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	$R3m$ (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	$R3m$ (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	$R3c$ (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	$R3c$ (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	$P\bar{3}1m$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		\bar{x}, \bar{y}, z	$2 \cdot 1 \cdot 2$
163	$P\bar{3}1c$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		\bar{x}, \bar{y}, z	$2 \cdot 1 \cdot 2$
164	$P\bar{3}m1$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		\bar{x}, \bar{y}, z	$2 \cdot 1 \cdot 2$
165	$P\bar{3}c1$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		\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	$P6$	P^16/mmm $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1622$	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$ $\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$ $0, 0, t$	$0, 0, 0$ /	y, x, z y, x, \bar{z}	$\infty \cdot 2 \cdot 2$ $\infty \cdot 2$
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 $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P^1622$	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$ $\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$ $0, 0, t$	$0, 0, 0$ /	y, x, z y, x, \bar{z}	$\infty \cdot 2 \cdot 2$ $\infty \cdot 2$
174	$P\bar{6}$	$P6/mmm$	$\frac{2}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, -\frac{1}{3}\mathbf{a} + \frac{1}{3}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{2}{3}, \frac{1}{3}, 0; 0, 0, \frac{1}{2}$	$0, 0, 0$	y, x, z	$6 \cdot 2 \cdot 2$
175	$P6/m$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
176	$P6_3/m$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
177	$P622$	$P6/mmm$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P622$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$ $\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$ $0, 0, \frac{1}{2}$	$0, 0, 0$ /		$2 \cdot 2 \cdot 1$ $2 \cdot 1$
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	$P6_322$	$P6/mmm$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P622$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$ $\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$ $0, 0, \frac{1}{2}$	$0, 0, 0$ /		$2 \cdot 2 \cdot 1$ $2 \cdot 1$
183	$P6mm$	P^16/mmm	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty \cdot 2 \cdot 1$
184	$P6cc$	P^16/mmm	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty \cdot 2 \cdot 1$

3.5. NORMALIZERS OF SPACE GROUPS

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	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty \cdot 2 \cdot 1$
186	$P6_3mc$	P^16/mmm	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0, 0, t$	$0, 0, 0$		$\infty \cdot 2 \cdot 1$
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	$P\bar{6}2m$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$0, 0, 0$		$2 \cdot 2 \cdot 1$
190	$P\bar{6}2c$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$	$0, 0, 0$		$2 \cdot 2 \cdot 1$
191	$P6/mmm$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
192	$P6/mcc$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
193	$P6_3/mcm$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
194	$P6_3/mmc$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, 0, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
195	$P23$	$Im\bar{3}m$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): I432$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$ $\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, 0$ /	y, x, z y, x, \bar{z}	$2 \cdot 2 \cdot 2$ $2 \cdot 2$
196	$F23$	$Im\bar{3}m$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): I432$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$ $\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$0, 0, 0$ /	y, x, z y, x, \bar{z}	$4 \cdot 2 \cdot 2$ $4 \cdot 2$
197	$I23$	$Im\bar{3}m$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): I432$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$ $\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ /	$0, 0, 0$ /	y, x, z y, x, \bar{z}	$1 \cdot 2 \cdot 2$ $1 \cdot 2$
198	$P2_13$	$Ia\bar{3}d$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): I4_132$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$ $\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, 0$ /	$y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	$2 \cdot 2 \cdot 2$ $2 \cdot 2$
199	$I2_13$	$Ia\bar{3}d$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): I4_132$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$ $\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ /	$0, 0, 0$ /	$y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$ $\bar{y} + \frac{1}{4}, \bar{x} + \frac{1}{4}, \bar{z} + \frac{1}{4}$	$1 \cdot 2 \cdot 2$ $1 \cdot 2$
200	$Pm\bar{3}$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
201	$Pn\bar{3} (23)$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
201	$Pn\bar{3} (\bar{3})$	$Im\bar{3}m (\bar{3}m)$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
202	$Fm\bar{3}$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
203	$Fd\bar{3} (23)$	$Pn\bar{3}m (\bar{4}3m)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
203	$Fd\bar{3} (\bar{3})$	$Pn\bar{3}m (\bar{3}m)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		y, x, z	$2 \cdot 1 \cdot 2$
204	$Im\bar{3}$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$			y, x, z	$1 \cdot 1 \cdot 2$
205	$Pa\bar{3}$	$Ia\bar{3}$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
206	$Ia\bar{3}$	$Ia\bar{3}d$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$		$y + \frac{1}{4}, x + \frac{1}{4}, z + \frac{1}{4}$	$1 \cdot 1 \cdot 2$
207	$P432$	$Im\bar{3}m$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): I432$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$ $\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, 0$ /		$2 \cdot 2 \cdot 1$ $2 \cdot 1$
208	$P4_232$	$Im\bar{3}m$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): I432$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$ $\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, 0$ /		$2 \cdot 2 \cdot 1$ $2 \cdot 1$
209	$F432$	$Pm\bar{3}m$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P432$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$ $\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, 0$ /		$2 \cdot 2 \cdot 1$ $2 \cdot 1$
210	$F4_132$	$Pn\bar{3}m (\bar{4}3m)$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): P4_232$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$ $\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ /		$2 \cdot 2 \cdot 1$ $2 \cdot 1$
211	$I432$	$Im\bar{3}m$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): I432$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$ $\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ /	$0, 0, 0$ /		$1 \cdot 2 \cdot 1$ $1 \cdot 1$
212	$P4_232$	$I4_132 [\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})]$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/		$2 \cdot 1$
213	$P4_132$	$I4_132 [\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})]$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	/		$2 \cdot 1$
214	$I4_132$	$Ia\bar{3}d$ $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}): I4_132$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$ $\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ /	$0, 0, 0$ /		$1 \cdot 2 \cdot 1$ $1 \cdot 1$
215	$P\bar{4}3m$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, 0$		$2 \cdot 2 \cdot 1$
216	$F\bar{4}3m$	$Im\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$0, 0, 0$		$4 \cdot 2 \cdot 1$
217	$I\bar{4}3m$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$		$0, 0, 0$		$1 \cdot 2 \cdot 1$
218	$P\bar{4}3n$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, 0$		$2 \cdot 2 \cdot 1$
219	$F\bar{4}3c$	$Im\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$0, 0, 0$		$4 \cdot 2 \cdot 1$
220	$I\bar{4}3d$	$Ia\bar{3}d$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$0, 0, 0$		$1 \cdot 2 \cdot 1$
221	$Pm\bar{3}n$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
222	$Pn\bar{3}n (432)$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
222	$Pn\bar{3}n (\bar{3})$	$Im\bar{3}m (\bar{3}m)$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
223	$Pm\bar{3}n$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$

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 · 1 · 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 · 1 · 1
225	$Fm\bar{3}m$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			2 · 1 · 1
226	$Fm\bar{3}c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			2 · 1 · 1
227	$Fd\bar{3}m$ ($\bar{4}3m$)	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			2 · 1 · 1
227	$Fd\bar{3}m$ ($\bar{3}m$)	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			2 · 1 · 1
228	$Fd\bar{3}c$ (23)	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			2 · 1 · 1
228	$Fd\bar{3}c$ ($\bar{3}$)	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$			2 · 1 · 1
229	$Im\bar{3}m$	$Im\bar{3}m$	a, b, c				1 · 1 · 1
230	$Ia\bar{3}d$	$Ia\bar{3}d$	a, b, c				1 · 1 · 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 $\bar{3}$ 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 ($\bar{2}$ 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.

3.5. NORMALIZERS OF SPACE GROUPS

Table 3.5.2.6

Affine normalizers of the triclinic and monoclinic space groups

Space group \mathcal{G}		Matrix-column pairs in Table 3.5.2.7	Space group \mathcal{G}		Matrix-column pairs in Table 3.5.2.7
No.	Hermann-Mauguin symbol		No.	Hermann-Mauguin symbol	
1	$P1$	M_1, v_1	9	$B11n$	$M_{10}, v_6; M_{15}, v_8$
2	$P\bar{1}$	M_1, v_2	9	$I11b$	$M_{10}, v_6; M_{11}, v_8$
3	$P121$	M_2, v_3	10	$P12/m1$	M_2, v_2
3	$P112$	M_3, v_4	10	$P112/m$	M_3, v_2
4	$P12_11$	M_2, v_3	11	$P12_1/m1$	M_2, v_2
4	$P112_1$	M_3, v_4	11	$P112_1/m$	M_3, v_2
5	$C121$	M_4, v_3	12	$C12/m1$	M_4, v_2
5	$A121$	M_5, v_3	12	$A12/m1$	M_5, v_2
5	$I121$	$M_6, v_3; M_7, v_3$	12	$I12/m1$	$M_6, v_2; M_7, v_2$
5	$A112$	M_8, v_4	12	$A112/m$	M_8, v_2
5	$B112$	M_9, v_4	12	$B112/m$	M_9, v_2
5	$I112$	$M_{10}, v_4; M_{11}, v_4$	12	$I112/m$	$M_{10}, v_2; M_{11}, v_2$
6	$P1m1$	M_2, v_5	13	$P12/c1$	M_5, v_2
6	$P11m$	M_3, v_6	13	$P12/n1$	$M_6, v_2; M_7, v_2$
7	$P1c1$	M_5, v_5	13	$P12/a1$	M_4, v_2
7	$P1n1$	$M_6, v_5; M_7, v_5$	13	$P112/a$	M_9, v_2
7	$P1a1$	M_4, v_5	13	$P112/n$	$M_{10}, v_2; M_{11}, v_2$
7	$P11a$	M_9, v_6	13	$P112/b$	M_8, v_2
7	$P11n$	$M_{10}, v_6; M_{11}, v_6$	14	$P12_1/c1$	M_5, v_2
7	$P11b$	M_8, v_6	14	$P12_1/n1$	$M_6, v_2; M_7, v_2$
8	$C1m1$	M_4, v_5	14	$P12_1/a1$	M_4, v_2
8	$A1m1$	M_5, v_5	14	$P112_1/a$	M_9, v_2
8	$I1m1$	$M_6, v_5; M_7, v_5$	14	$P112_1/n$	$M_{10}, v_2; M_{11}, v_2$
8	$A11m$	M_8, v_6	14	$P112_1/b$	M_8, v_2
8	$B11m$	M_9, v_6	15	$C12/c1$	$M_6, v_2; M_{12}, v_9$
8	$I11m$	$M_{10}, v_6; M_{11}, v_6$	15	$A12/n1$	$M_6, v_2; M_{13}, v_{10}$
9	$C1c1$	$M_6, v_5; M_{12}, v_7$	15	$I12/a1$	$M_6, v_2; M_7, v_{11}$
9	$A1n1$	$M_6, v_5; M_{13}, v_7$	15	$A112/a$	$M_{10}, v_2; M_{14}, v_{10}$
9	$I1a1$	$M_6, v_5; M_7, v_7$	15	$B112/n$	$M_{10}, v_2; M_{15}, v_{12}$
9	$A11a$	$M_{10}, v_6; M_{14}, v_8$	15	$I112/b$	$M_{10}, v_2; M_{11}, v_{11}$

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, $\det(M_i) = \pm 1$ must hold.

$M_1 = \begin{pmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{pmatrix}$	$M_2 = \begin{pmatrix} n_{11} & 0 & n_{13} \\ 0 & \pm 1 & 0 \\ n_{31} & 0 & n_{33} \end{pmatrix}$	$M_3 = \begin{pmatrix} n_{11} & n_{12} & 0 \\ n_{21} & n_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$	$M_4 = \begin{pmatrix} u_{11} & 0 & n_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{pmatrix}$	$M_5 = \begin{pmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ n_{31} & 0 & u_{33} \end{pmatrix}$
$M_6 = \begin{pmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{pmatrix}$	$M_7 = \begin{pmatrix} g_{11} & 0 & u_{13} \\ 0 & \pm 1 & 0 \\ u_{31} & 0 & g_{33} \end{pmatrix}$	$M_8 = \begin{pmatrix} u_{11} & g_{12} & 0 \\ n_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$	$M_9 = \begin{pmatrix} u_{11} & n_{12} & 0 \\ g_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$	$M_{10} = \begin{pmatrix} u_{11} & g_{12} & 0 \\ g_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$
$M_{11} = \begin{pmatrix} g_{11} & u_{12} & 0 \\ u_{21} & g_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$	$M_{12} = \begin{pmatrix} u_{11} & 0 & u_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{pmatrix}$	$M_{13} = \begin{pmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ u_{31} & 0 & u_{33} \end{pmatrix}$	$M_{14} = \begin{pmatrix} u_{11} & g_{12} & 0 \\ u_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$	$M_{15} = \begin{pmatrix} u_{11} & u_{12} & 0 \\ g_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$
$v_1 = \begin{pmatrix} r \\ s \\ t \end{pmatrix}$	$v_2 = \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \\ \frac{1}{2}n_3 \end{pmatrix}$	$v_3 = \begin{pmatrix} \frac{1}{2}n_1 \\ s \\ \frac{1}{2}n_3 \end{pmatrix}$	$v_4 = \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \\ t \end{pmatrix}$	$v_5 = \begin{pmatrix} r \\ \frac{1}{2}n_2 \\ t \end{pmatrix}$
$v_6 = \begin{pmatrix} r \\ s \\ \frac{1}{2}n_3 \end{pmatrix}$	$v_7 = \begin{pmatrix} r \\ \frac{1}{4}u_2 \\ t \end{pmatrix}$	$v_8 = \begin{pmatrix} r \\ s \\ \frac{1}{4}u_3 \end{pmatrix}$	$v_9 = \begin{pmatrix} \frac{1}{4}u_1 \\ \frac{1}{4}u_2 \\ \frac{1}{2}n_3 \end{pmatrix}$	$v_{10} = \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{4}u_2 \\ \frac{1}{4}u_3 \end{pmatrix}$
$v_{11} = \begin{pmatrix} \frac{1}{4}u_1 \\ \frac{1}{4}u_2 \\ \frac{1}{4}u_3 \end{pmatrix}$	$v_{12} = \begin{pmatrix} \frac{1}{4}u_1 \\ \frac{1}{2}n_2 \\ \frac{1}{4}u_3 \end{pmatrix}$			

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 $z = 0.515$. $\mathcal{N}_{\mathcal{E}}(P4mm) = P^4/mmm$ ($\frac{1}{2}(\mathbf{a} - \mathbf{b}), \frac{1}{2}(\mathbf{a} + \mathbf{b}), \varepsilon\mathbf{c}$) 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 enantiomorphic 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 $\not{4}_322$ (rod group of the molecules, not imposed by the space group; Schnering & Hönle, 1979). The chains wind round 2_1 axes parallel to \mathbf{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 $\not{4}_322$ helices to the enantiomorphic right-handed $\not{4}_122$ 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 \mathbf{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

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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 $|F(\mathbf{h})|$, but they differ in their indices $\mathbf{h} = (h, k, l)$ and phases $\varphi(\mathbf{h})$.

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 (\mathbf{P}, \mathbf{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:

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

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

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 \mathbf{h} of all structure factors unchanged but transform their phases according to $\varphi'(\mathbf{h}) = \varphi(\mathbf{h}) - 2\pi\mathbf{h}\mathbf{p}$. 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 \mathbf{h} to $\mathbf{h}' = -\mathbf{h}$, 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 \mathbf{h} and $-\mathbf{h}$ 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 $\mathbf{p} \neq \mathbf{o}$. The choice between these equivalent descriptions of the crystal

Table 3.5.3.1

Changes of structure-factor phases for the equivalent descriptions of a crystal structure in $F222$

F222	$h + k + l =$			
	$4n$	$4n + 2$	$4n + 1$	$4n + 3$
$t(0, 0, 0)$	$\varphi(\mathbf{h})$	$\varphi(\mathbf{h})$	$\varphi(\mathbf{h})$	$\varphi(\mathbf{h})$
$t(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$	$\varphi(\mathbf{h})$	$\pi + \varphi(\mathbf{h})$	$\frac{3}{2}\pi + \varphi(\mathbf{h})$	$\frac{1}{2}\pi + \varphi(\mathbf{h})$
$t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$\varphi(\mathbf{h})$	$\varphi(\mathbf{h})$	$\pi + \varphi(\mathbf{h})$	$\pi + \varphi(\mathbf{h})$
$t(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$	$\varphi(\mathbf{h})$	$\pi + \varphi(\mathbf{h})$	$\frac{1}{2}\pi + \varphi(\mathbf{h})$	$\frac{3}{2}\pi + \varphi(\mathbf{h})$
$\bar{1} 0, 0, 0$	$-\varphi(\mathbf{h})$	$-\varphi(\mathbf{h})$	$-\varphi(\mathbf{h})$	$-\varphi(\mathbf{h})$
$\bar{1} \frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$-\varphi(\mathbf{h})$	$\pi - \varphi(\mathbf{h})$	$\frac{1}{2}\pi - \varphi(\mathbf{h})$	$\frac{3}{2}\pi - \varphi(\mathbf{h})$
$\bar{1} \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$-\varphi(\mathbf{h})$	$-\varphi(\mathbf{h})$	$\pi - \varphi(\mathbf{h})$	$\pi - \varphi(\mathbf{h})$
$\bar{1} \frac{3}{8}, \frac{3}{8}, \frac{3}{8}$	$-\varphi(\mathbf{h})$	$\pi - \varphi(\mathbf{h})$	$\frac{3}{2}\pi - \varphi(\mathbf{h})$	$\frac{1}{2}\pi - \varphi(\mathbf{h})$

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.

Example

According to Table 3.5.2.4, eight equivalent descriptions exist for each crystal structure with symmetry $F222$. 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 $\varphi'(\mathbf{h}) = \varphi(\mathbf{h}) - (\pi/2)(h + k + l)$, 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 $\varphi(\mathbf{h}_1)$ to a range of length $\pi/2$ fixes the origin. Restriction of a second phase $\varphi(\mathbf{h}_2)$ 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 $\varphi'(\mathbf{h}) = -\varphi(\mathbf{h})$. 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 $\varphi(\mathbf{h}_2)$ 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 $\varphi(\mathbf{h}_1)$ and $\varphi(\mathbf{h}_2)$ and, moreover, on the range chosen for $\varphi(\mathbf{h}_1)$. If, for instance, $\varphi(\mathbf{h}_1)$ with $h + k + l = 4n + 1$ is restricted to $\pi/2 \leq \varphi(\mathbf{h}_1) < \pi$, one of the following restrictions may be chosen for $\varphi(\mathbf{h}_2)$: $0 < \varphi(\mathbf{h}_2) < \pi$ for $h + k + l = 4n$; $-\pi/2 < \varphi(\mathbf{h}_2) < \pi/2$ for $h + k + l = 4n + 2$; $-\pi/4 < \varphi(\mathbf{h}_2) < 3\pi/4$ for $h + k + l = 4n + 1$; $-3\pi/4 < \varphi(\mathbf{h}_2) < \pi/4$ for $h + k + l = 4n + 3$. If, however, the phase $\varphi(\mathbf{h}_1)$ of the same first reflection was restricted to $-\pi/4 \leq \varphi(\mathbf{h}_1) < 3\pi/4$, the possible restrictions for the second phase change to: $0 < \varphi(\mathbf{h}_2) < \pi$ for $h + k + l = 4n$ or $4n + 2$; $-\pi/2 < \varphi(\mathbf{h}_2) < \pi/2$ 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, 1984b):

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 (super-groups)’ 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) $\mathcal{G} = Pmma$ ($\mathbf{a}, \mathbf{b}, \mathbf{c}$), $\mathcal{H} = Pmmm$ ($\mathbf{a}, 2\mathbf{b}, \mathbf{c}$).

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 $\mathcal{N}_{\mathcal{A}}(Pmmm) = P4/mmm$ ($\frac{1}{2}\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$) is the group $\mathcal{M}(Pmma, Pmmm) = Pmmm$ ($\frac{1}{2}\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$), which is a proper subgroup of both normalizers. As i_g equals 2, $Pmma$ has two affine-equivalent subgroups of type $Pmmm$ 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, $Pmmm$ 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, 1984a) 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 $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = \mathcal{N}_{\mathcal{A}}(\mathcal{G}) = P^4/mmm$ ($\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$) 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 $\mathcal{N}_{\mathcal{A}}(P112/m)$.

3.5.4. Normalizers of point groups

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References

Normalizers with respect to the Euclidean or affine group may be defined for any group of isometries (*cf.* Gubler, 1982a,b). For a point group, however, it seems inadequate to use a supergroup that contains transformations that do not map a fixed point of that point group onto itself. Appropriate supergroups for the definition of normalizers of point groups are the full isometry groups of the sphere, $m\infty$, and of the circle, ∞m , in three-dimensional and two-dimensional space (*cf.* Galiulin, 1978).

These normalizers are listed in Tables 3.5.4.1 and 3.5.4.2. It has to be noticed that the normalizer of a crystallographic point group may contain continuous rotations, *i.e.* rotations with infinitesimal rotation angle, or noncrystallographic rotations (∞m ; $m\infty$, ∞/mm , $8mm$, $12mm$; $8/mmm$, $12/mmm$). In analogy to space groups, these normalizers define equivalence relationships on the 'Wyckoff positions' of the point groups (*cf.* Sections 3.2.3 and 3.2.4). They give also the relation between the different but equivalent morphological descriptions of a crystal.

Table 3.5.4.1

Normalizers of the two-dimensional point groups with respect to the full isometry group of the circle

The upper part refers to the crystallographic, the lower part to the noncrystallographic point groups as listed in Table 3.2.1.5. The letter n represents an arbitrary integer; $(2n)$ represents an even number.

Normalizer	Point groups
∞m	1, 2, 4, 3, 6
$12mm$	$6mm$
$8mm$	$4mm$
$6mm$	$3m$
$4mm$	$2mm$
$2mm$	m
∞m	$n, \infty, \infty m$
$(2n)mm$	nmm, nm

Table 3.5.4.2

Normalizers of the three-dimensional point groups with respect to the full isometry group of the sphere

The upper part refers to the crystallographic, the lower part to the noncrystallographic point groups as listed in Table 3.2.1.6. The letter n represents an arbitrary integer; $(2n)$ represents an even number.

Normalizer	Point groups
$m\infty$	1, $\bar{1}$
$m\bar{3}m$	222, mmm , 23, $m\bar{3}$, 432, $\bar{4}3m$, $m\bar{3}m$
∞/mm	2, m , $2/m$, 4, $\bar{4}$, $4/m$, 3, $\bar{3}$, 6, $\bar{6}$, $6/m$
$12/mmm$	622, $6mm$, $6/mmm$
$8/mmm$	422, $4mm$, $4/mmm$
$6/mmm$	32, $3m$, $\bar{3}m$, $\bar{6}2m$
$4/mmm$	$mm2$, $\bar{4}2m$
$m\infty$	2∞ , $m\infty$
$m\bar{3}5$	235, $m\bar{3}5$
∞/mm	$n, \bar{n}, n/m, \infty, \infty/m, \infty 2, \infty m, \infty/mm$
$(2n)/mmm$	$n22, nmm, n/mmm, n2, nm, \bar{n}m$
n/mmm	$\bar{n}2m$

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