

## 15.2. Euclidean and affine normalizers of plane groups and space groups

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### 15.2.1. 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: *Pmmm* 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. 15.2.1.1 to 15.2.1.4 are based on these studies.

Fig. 15.2.1.1 shows a suitably chosen parameter region for the five space-group types *P2*, *P2<sub>1</sub>*, *Pm*, *P2/m* and *P2<sub>1</sub>/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 intersection 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<sub>1</sub>/c* and *C2/c*, and for each setting three possibilities of cell choice are listed in Part 7, which can be distinguished by different space-group symbols (example: *C12/m1*,

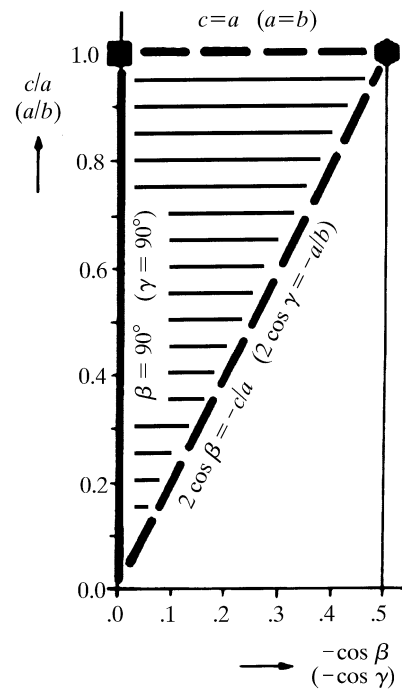


Fig. 15.2.1.1. Parameter range for space groups of types *P2*, *P2<sub>1</sub>*, *Pm*, *P2/m* and *P2<sub>1</sub>/m* (plane groups of types *p1* and *p2*). The information in parentheses refers to unique axis *c*.

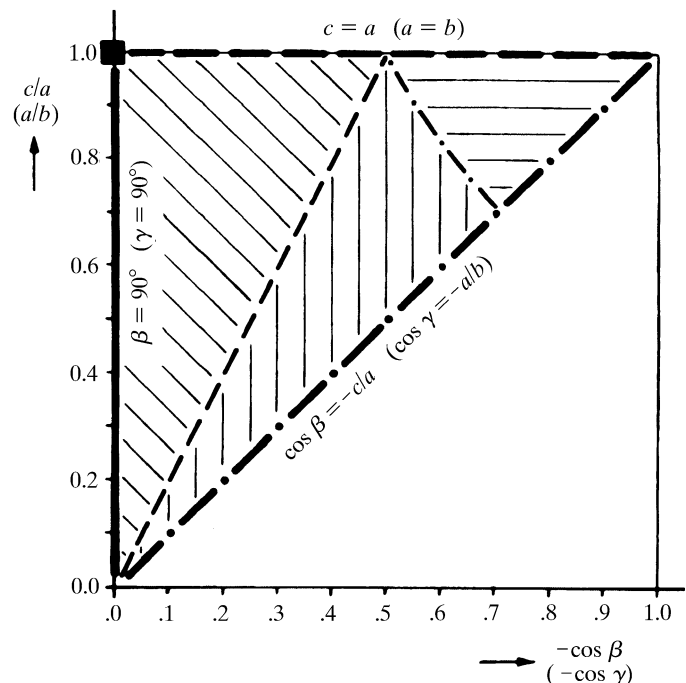


Fig. 15.2.1.2. Parameter range for space groups of types *C2*, *Pc*, *Cm*, *Cc*, *C2/m*, *P2/c*, *P2<sub>1</sub>/c* and *C2/c*:  
 unique axis *b*, cell choice 2: *P1n1*, *P12/n1*, *P12<sub>1</sub>/n1*;  
 unique axis *b*, cell choice 3: *I121*, *I1m1*, *I1a1*, *I12/m1*, *I12/a1*;  
 unique axis *c*, cell choice 2: *P11n*, *P112/n*, *P112<sub>1</sub>/n*;  
 unique axis *c*, cell choice 3: *I112*, *I11m*, *I11b*, *I112/m*, *I112/b*.  
 The information in parentheses refers to unique axis *c*.

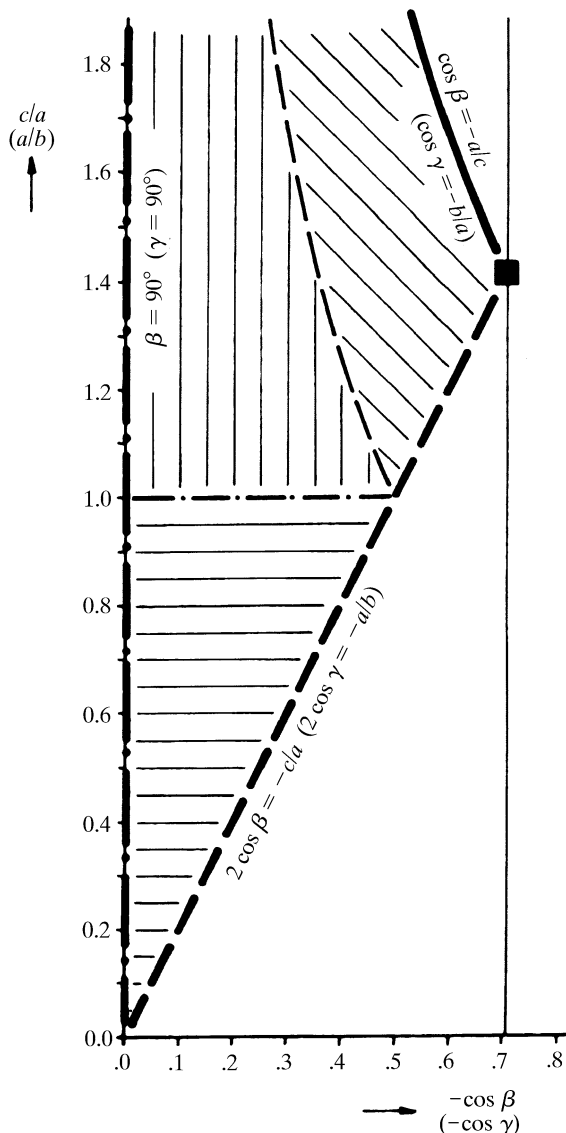


Fig. 15.2.1.3. Parameter range for space groups of types  $C2$ ,  $Pc$ ,  $Cm$ ,  $Cc$ ,  $C2/m$ ,  $P2/c$ ,  $P2_1/c$  and  $C2/c$ :

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  $c$ .

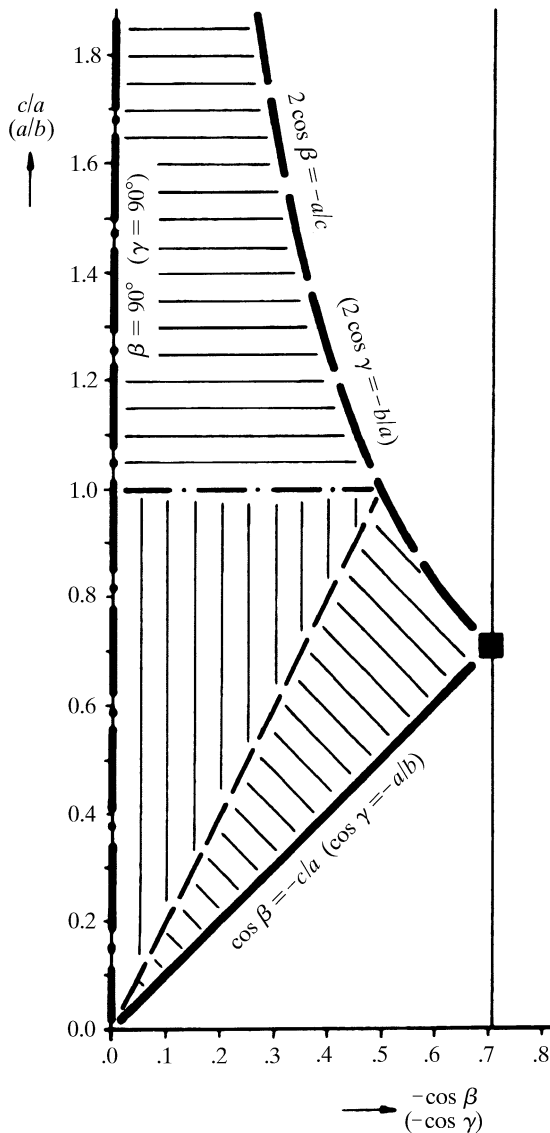


Fig. 15.2.1.4. Parameter range for space groups of types  $C2$ ,  $Pc$ ,  $Cm$ ,  $Cc$ ,  $C2/m$ ,  $P2/c$ ,  $P2_1/c$  and  $C2/c$ :

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  $c$ .

$A12/m1$ ,  $I12/m1$ ,  $A112/m$ ,  $B112/m$ ,  $I112/m$ ). 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. 15.2.1.2, 15.2.1.3 or 15.2.1.4) is larger than the range shown in Fig. 15.2.1.1 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. 15.2.1.2 to 15.2.1.4. 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. 15.2.1.1, 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

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

holds.  $\mathcal{K}(\mathcal{G})$  is that class-equivalent supergroup of  $\mathcal{G}$  that is at the same time a translation-equivalent subgroup of  $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ . It is well defined according to a 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

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Table 15.2.1.1. Euclidean normalizers of the plane groups

For the restrictions of the cell metric of the two oblique plane groups see text and Fig. 15.2.1.3.

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	$p^2$	$\varepsilon_1 \mathbf{a}, \varepsilon_2 \mathbf{b}$	$r, 0; 0, s$	$-x, -y$		$\infty^2 \cdot 2 \cdot 1$
		$a < b, \gamma = 90^\circ$	$p^2 2mm$	$\varepsilon_1 \mathbf{a}, \varepsilon_2 \mathbf{b}$	$r, 0; 0, s$	$-x, -y$	$-x, y$	$\infty^2 \cdot 2 \cdot 2$
		$2 \cos \gamma = -a/b, 90 < \gamma < 120^\circ$	$c^2 2mm$	$\varepsilon_1 \mathbf{a}, \varepsilon_2 (\frac{1}{2} \mathbf{a} + \mathbf{b})$	$r, 0; 0, s$	$-x, -y$	$x - y, -y$	$\infty^2 \cdot 2 \cdot 2$
		$a = b, 90 < \gamma < 120^\circ$	$c^2 2mm$	$\varepsilon_1 (\mathbf{a} - \mathbf{b}), \varepsilon_2 (\mathbf{a} + \mathbf{b})$	$r, 0; 0, s$	$-x, -y$	$y, x$	$\infty^2 \cdot 2 \cdot 2$
		$a = b, \gamma = 90^\circ$	$p^2 4mm$	$\varepsilon \mathbf{a}, \varepsilon \mathbf{b}$	$r, 0; 0, s$	$-x, -y$	$-x, y; y, x$	$\infty^2 \cdot 2 \cdot 4$
		$a = b, \gamma = 120^\circ$	$p^2 6mm$	$\varepsilon \mathbf{a}, \varepsilon \mathbf{b}$	$r, 0; 0, s$	$-x, -y$	$y, x; x, x - y$	$\infty^2 \cdot 2 \cdot 6$
2	$p2$	General	$p2$	$\frac{1}{2} \mathbf{a}, \frac{1}{2} \mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a < b, \gamma = 90^\circ$	$p2mm$	$\frac{1}{2} \mathbf{a}, \frac{1}{2} \mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$-x, y$	$4 \cdot 1 \cdot 2$
		$2 \cos \gamma = -a/b, 90 < \gamma < 120^\circ$	$c2mm$	$\frac{1}{2} \mathbf{a}, \frac{1}{2} \mathbf{a} + \mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$x - y, -y$	$4 \cdot 1 \cdot 2$
		$a = b, 90 < \gamma < 120^\circ$	$c2mm$	$\frac{1}{2} (\mathbf{a} - \mathbf{b}), \frac{1}{2} (\mathbf{a} + \mathbf{b})$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$y, x$	$4 \cdot 1 \cdot 2$
		$a = b, \gamma = 90^\circ$	$p4mm$	$\frac{1}{2} \mathbf{a}, \frac{1}{2} \mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$-x, y; y, x$	$4 \cdot 1 \cdot 4$
		$a = b, \gamma = 120^\circ$	$p6mm$	$\frac{1}{2} \mathbf{a}, \frac{1}{2} \mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$y, x; x, x - y$	$4 \cdot 1 \cdot 6$
3	$p1m1$	$a \neq b$ $a = b$	$p^1 2mm$	$\frac{1}{2} \mathbf{a}, \varepsilon \mathbf{b}$	$\frac{1}{2}, 0; 0, s$	$-x, -y$		$(2 \cdot \infty) \cdot 2 \cdot 1$
4	$p1g1$		$p^1 2mm$	$\frac{1}{2} \mathbf{a}, \varepsilon \mathbf{b}$	$\frac{1}{2}, 0; 0, s$	$-x, -y$		$(2 \cdot \infty) \cdot 2 \cdot 1$
5	$c1m1$		$p^1 2mm$	$\frac{1}{2} \mathbf{a}, \varepsilon \mathbf{b}$	$0, s$	$-x, -y$		$\infty \cdot 2 \cdot 1$
6	$p2mm$		$p2mm$	$\frac{1}{2} \mathbf{a}, \frac{1}{2} \mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
			$p4mm$	$\frac{1}{2} \mathbf{a}, \frac{1}{2} \mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		$y, x$	$4 \cdot 1 \cdot 2$
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	$p6mm$		$p6mm$	$\mathbf{a}, \mathbf{b}$				$1 \cdot 1 \cdot 1$

Laue class of  $\mathcal{G}$ . If  $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$  is noncentrosymmetric, an intermediate group  $\mathcal{L}(\mathcal{G})$  cannot exist.

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 15.2.1.1, those of triclinic space groups in Table 15.2.1.2, of monoclinic and orthorhombic space groups in Table 15.2.1.3, and those of all other space groups in Table 15.2.1.4. Herein all settings and choices of cell and origin as tabulated in Parts 6 and 7 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 15.2.1.3.)

The first column of Tables 15.2.1.1, 15.2.1.3 and 15.2.1.4 shows the number of the plane group or space group, the second column its Hermann–Mauguin symbol together with information on the setting, cell choice and origin, if necessary. Special metrical conditions affecting the Euclidean normalizer are tabulated in the third column of Tables 15.2.1.1 and 15.2.1.3. The term ‘general’ means that only the general metrical conditions for the respective crystal system are valid. In Table 15.2.1.4, 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 Table 15.2.1.3 (15.2.1.1) or in the third column of Table 15.2.1.4. 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

## 15. NORMALIZERS OF SPACE GROUPS AND THEIR USE IN CRYSTALLOGRAPHY

Table 15.2.1.2. *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 $\mathcal{N}_E(\mathcal{G})$ of	
	1	2
$aP$	$P^3\bar{1}$	$P\bar{1}$
$mP$	$P^32/m$	$P2/m$
$mA$	$P^32/m$	$A2/m$
$oP$	$P^3mmm$	$Pmmm$
$oC$	$P^3mmm$	$Cmmm$
$oF$	$P^3mmm$	$Fmmm$
$oI$	$P^3mmm$	$Immm$
$tP$	$P^34/mmm$	$P4/mmm$
$tI$	$P^34/mmm$	$I4/mmm$
$hP$	$P^36/mmm$	$P6/mmm$
$hR$	$P^3\bar{3}m1$	$R\bar{3}m$
$cP$	$P^3m\bar{3}m$	$Pm\bar{3}m$
$cF$	$P^3m\bar{3}m$	$Fm\bar{3}m$
$cI$	$P^3m\bar{3}m$	$Im\bar{3}m$

$P^3$  ( $p^1, c^1, p^2$ ), respectively, are used instead of the Bravais letter.\* Setting and origin choice for the Euclidean normalizers are indicated as for space groups. In a few cases, origin choices not tabulated in Part 7 are needed.

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

The following three columns specify a set of additional symmetry operations that generate  $\mathcal{K}(\mathcal{G})$ ,  $\mathcal{L}(\mathcal{G})$  and  $\mathcal{N}_E(\mathcal{G})$  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  $\mathcal{N}_E(\mathcal{G})$  is centrosymmetric, the position of an additional centre of symmetry 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.) If, however,  $\mathcal{N}_E(\mathcal{G})$  is noncentrosymmetric and, therefore,  $\mathcal{L}(\mathcal{G})$  is undefined, this fact is indicated by a slash. The last of these columns contains entries only if  $\mathcal{G}$  and  $\mathcal{N}_E(\mathcal{G})$  belong to different Laue classes. The corresponding additional generators are listed as coordinate triplets.

In the last column, the subgroup index of  $\mathcal{G}$  in  $\mathcal{N}_E(\mathcal{G})$  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  $\mathcal{N}_E(\mathcal{G})$ . [In the case of a noncentrosymmetric normalizer, the index of  $\mathcal{G}$  in  $\mathcal{N}_E(\mathcal{G})$  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  $\mathcal{N}_E(\mathcal{G})$ .] For continuous translations,  $k_g$  is always infinite. Nevertheless, it is useful to distinguish different cases:  $\infty, \infty^2$  and  $\infty^3$  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 Part 9 and literature on 'reduced cells' cited

therein). Table 15.2.1.2 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 inherent symmetry 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  $P\bar{1}$ .

### 15.2.2. 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  $\mathcal{N}_E(\mathcal{G})$ , or both normalizers coincide:

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

As any translation is an isometry, each translation belonging to  $\mathcal{N}_A(\mathcal{G})$  also belongs to  $\mathcal{N}_E(\mathcal{G})$ . 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 normalizers are identical, irrespective of any metrical specialization, *i.e.*  $\mathcal{N}_E(\mathcal{G}) = \mathcal{N}_A(\mathcal{G})$  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 2 further rectangular types) [examples:  $\mathcal{N}_A(Pcca) = Pmmm$ ,  $\mathcal{N}_A(Pnc2) = P^1mmm$ ].

For each of the other 38 types of orthorhombic space group (5 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:  $\mathcal{N}_A(Pbca) = Pm\bar{3}$ ,  $\mathcal{N}_A(Pccn) = P4/mmm$ ,  $\mathcal{N}_A(Pcc2) = P^14/mmm$ ].

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–vector 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 (1982a,b).

In Table 15.2.2.1, the affine normalizers of all triclinic and monoclinic space groups are given. The first two columns correspond to those of Table 15.2.1.3 or 15.2.1.4. The affine normalizers are completely described in column 3 by one or two general matrix–vector pairs. All unimodular matrices and vectors used in Table 15.2.2.1 are listed explicitly in Table 15.2.2.2. The matrix–vector representation of an affine normalizer consists of all

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

(continued on page 894)