

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	$p2mm$		$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
			$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$		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	$c2mm$		$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0; 0, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
		$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0$		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-