

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

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 $\mathcal{N}_E(\mathcal{G})$ 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 $\mathcal{N}_E(\mathcal{G})$ 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 $\mathcal{N}_E(\mathcal{G})$ or $\mathcal{N}_{E^+}(\mathcal{G})$ 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 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 $\mathcal{N}_{E^+}(\mathcal{G})$ and also if $\mathcal{N}_E(\mathcal{G})$ 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 $\mathcal{N}_E(\mathcal{G})$ or $\mathcal{N}_{E^+}(\mathcal{G})$.

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 $\mathcal{N}_{E^+}(\mathcal{G})$ or $\mathcal{N}_{E^+}(\mathcal{G})$.] 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 $\mathcal{N}_E(\mathcal{G})$, 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 normalizer 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 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.

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