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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

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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, 2*mm*, 3, 3*m*, 4, 4*mm*, 6 and 6*mm*, 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. 3.5.2.1 to 3.5.2.4 are based on these studies.

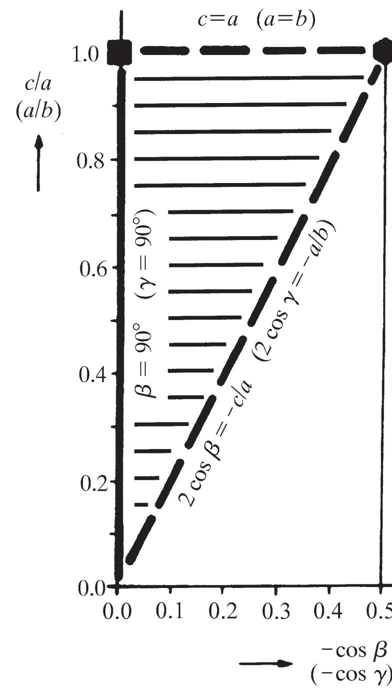

Figure 3.5.2.1
Parameter range for space groups of types $P2, P2_1, Pm, P2/m$ and $P2_1/m$ (plane groups of types $p1$ and $p2$). The information in parentheses refers to unique axis *c*.

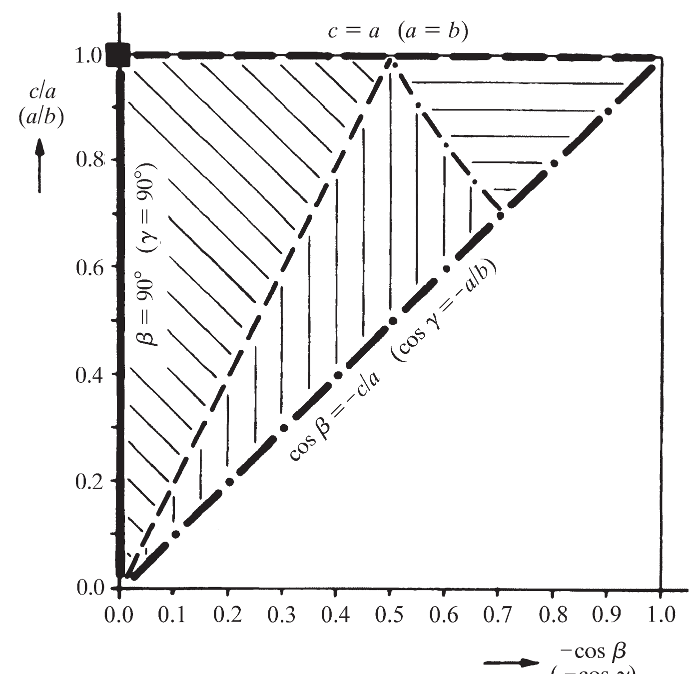

Figure 3.5.2.2
Parameter range for space groups of types $C2$, Pc, Cm, Cc, $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$. They refer to the following settings:
unique axis *b*, cell choice 2: $P1n1$, $P12/n1$, $P12_1/n1$;
unique axis *b*, cell choice 3: $I121$, $I1m1$, $I1a1$, $I12/m1$, $I12/a1$;
unique axis *c*, 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-