

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

BY E. KOCH, W. FISCHER AND U. MÜLLER

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 $P2$, $P2_1$, 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 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 , $C2/m$, $P2/c$, $P2_1/c$ 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: $C12/m_1$,

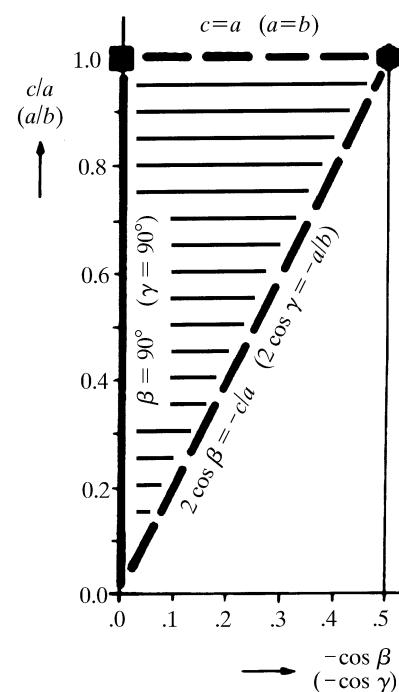


Fig. 15.2.1.1. Parameter range for space groups of types $P2$, $P2_1$, Pm , $P2/m$ and $P2_1/m$ (plane groups of types $p1$ and $p2$). The information in parentheses refers to unique axis c .

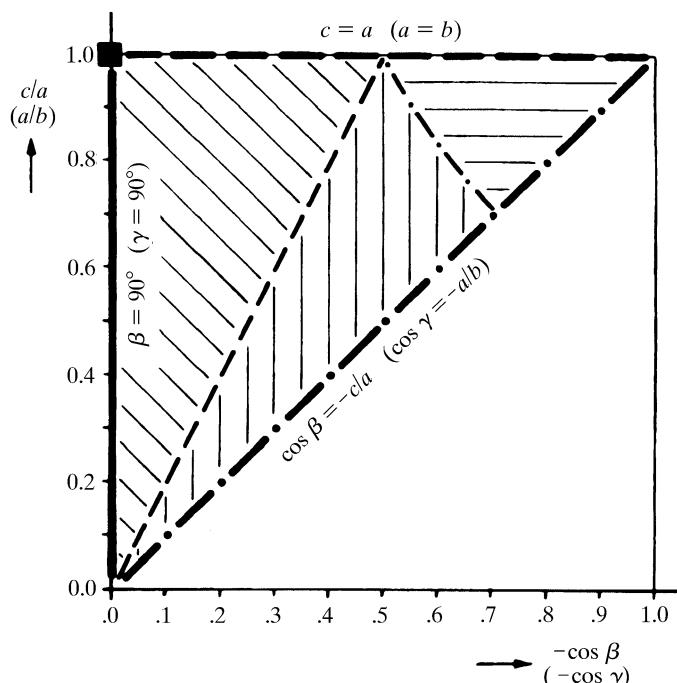


Fig. 15.2.1.2. Parameter range for space groups of types $C2$, Pc , Cm , Cc , $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$:
unique axis b , cell choice 2: $P1n1$, $P12/n1$, $P12_1/n1$;
unique axis b , cell choice 3: $I121$, $I1m1$, $I1a1$, $I12/m1$, $I12/a1$;
unique axis c , cell choice 2: $P11n$, $P112/n$, $P112_1/n$;
unique axis c , cell choice 3: $I112$, $I11m$, $I11b$, $I112/m$, $I112/b$.
The information in parentheses refers to unique axis c .