

## 3.5. NORMALIZERS OF SPACE GROUPS

## 3.5.4. Normalizers of point groups

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## References

Normalizers with respect to the Euclidean or affine group may be defined for any group of isometries (*cf.* Gubler, 1982a,b). For a point group, however, it seems inadequate to use a supergroup that contains transformations that do not map a fixed point of that point group onto itself. Appropriate supergroups for the definition of normalizers of point groups are the full isometry groups of the sphere,  $m\infty$ , and of the circle,  $\infty m$ , in three-dimensional and two-dimensional space (*cf.* Galiulin, 1978).

These normalizers are listed in Tables 3.5.4.1 and 3.5.4.2. It has to be noticed that the normalizer of a crystallographic point group may contain continuous rotations, *i.e.* rotations with infinitesimal rotation angle, or noncrystallographic rotations ( $\infty m$ ;  $m\infty$ ,  $\infty/mm$ ,  $8mm$ ,  $12mm$ ;  $8/mmm$ ,  $12/mmm$ ). In analogy to space groups, these normalizers define equivalence relationships on the 'Wyckoff positions' of the point groups (*cf.* Sections 3.2.3 and 3.2.4). They give also the relation between the different but equivalent morphological descriptions of a crystal.

**Table 3.5.4.1**

Normalizers of the two-dimensional point groups with respect to the full isometry group of the circle

The upper part refers to the crystallographic, the lower part to the noncrystallographic point groups as listed in Table 3.2.1.5. The letter  $n$  represents an arbitrary integer;  $(2n)$  represents an even number.

Normalizer	Point groups
$\infty m$	1, 2, 4, 3, 6
$12mm$	$6mm$
$8mm$	$4mm$
$6mm$	$3m$
$4mm$	$2mm$
$2mm$	$m$
$\infty m$	$n, \infty, \infty m$
$(2n)mm$	$nmm, nm$

**Table 3.5.4.2**

Normalizers of the three-dimensional point groups with respect to the full isometry group of the sphere

The upper part refers to the crystallographic, the lower part to the noncrystallographic point groups as listed in Table 3.2.1.6. The letter  $n$  represents an arbitrary integer;  $(2n)$  represents an even number.

Normalizer	Point groups
$m\infty$	1, $\bar{1}$
$m\bar{3}m$	222, $mmm$ , 23, $m\bar{3}$ , 432, $\bar{4}3m$ , $m\bar{3}m$
$\infty/mm$	2, $m$ , $2/m$ , 4, $\bar{4}$ , $4/m$ , 3, $\bar{3}$ , 6, $\bar{6}$ , $6/m$
$12/mmm$	622, $6mm$ , $6/mmm$
$8/mmm$	422, $4mm$ , $4/mmm$
$6/mmm$	32, $3m$ , $\bar{3}m$ , $\bar{6}2m$
$4/mmm$	$mm2$ , $\bar{4}2m$
$m\infty$	$2\infty, m\infty$
$m\bar{3}5$	235, $m\bar{3}5$
$\infty/mm$	$n, \bar{n}, n/m, \infty, \infty/m, \infty 2, \infty m, \infty/mm$
$(2n)/mmm$	$n22, nmm, n/mmm, n2, nm, \bar{n}m$
$n/mmm$	$\bar{n}2m$

- Billiet, Y., Burzlaff, H. & Zimmermann, H. (1982). *Comment on the paper of H. Burzlaff and H. Zimmermann. 'On the choice of origin in the description of space groups'*. *Z. Kristallogr.* **160**, 155–157.
- Burzlaff, H. & Zimmermann, H. (1980). *On the choice of origin in the description of space groups*. *Z. Kristallogr.* **153**, 151–179.
- Buttner, R. H. & Maslen, E. N. (1992). *Structural parameters and electron difference density in BaTiO<sub>3</sub>*. *Acta Cryst.* **B48**, 764–769.
- Fischer, W. (1968). *Kreispackungsbedingungen in der Ebene*. *Acta Cryst.* **A24**, 67–81.
- Fischer, W. (1971). *Existenzbedingungen homogener Kugelpackungen in Raumgruppen tetragonaler Symmetrie*. *Z. Kristallogr.* **133**, 18–42.
- Fischer, W. (1991). *Tetragonal sphere packings II. Lattice complexes with two degrees of freedom*. *Z. Kristallogr.* **194**, 87–110.
- Fischer, W. & Koch, E. (1983). *On the equivalence of point configurations due to Euclidean normalizers (Cheshire groups) of space groups*. *Acta Cryst.* **A39**, 907–915.
- Flack, H. D. (2003). *Chiral and achiral crystal structures*. *Helv. Chim. Acta*, **86**, 905–921.
- Galiulin, R. V. (1978). *Holohedral varieties of simple forms of crystals*. *Sov. Phys. Crystallogr.* **23**, 635–641; *Kristallografiya*, **53**, 1125–1132.
- Gubler, M. (1982a). *Über die Symmetrien der Symmetriegruppen: Automorphismengruppen, Normalisatorgruppen und charakteristische Untergruppen von Symmetriegruppen, insbesondere der kristallographischen Punkt- und Raumgruppen*. Dissertation, University of Zürich, Switzerland.
- Gubler, M. (1982b). *Normalizer groups and automorphism groups of symmetry groups*. *Z. Kristallogr.* **158**, 1–26.
- Hermann, C. (1929). *Zur systematischen Strukturtheorie. IV. Untergruppen*. *Z. Kristallogr.* **69**, 533–555.
- Hirshfeld, F. L. (1968). *Symmetry in the generation of trial structures*. *Acta Cryst.* **A24**, 301–311.
- Koch, E. (1984a). *A geometrical classification of cubic point configurations*. *Z. Kristallogr.* **166**, 23–52.
- Koch, E. (1984b). *The implications of normalizers on group-subgroup relations between space groups*. *Acta Cryst.* **A40**, 593–600.
- Koch, E. (1986). *Implications of Euclidean normalizers of space groups in reciprocal space*. *Cryst. Res. Technol.* **21**, 1213–1219.
- Koch, E. & Fischer, W. (1975). *Automorphismengruppen von Raumgruppen und die Zuordnung von Punktlagen zu Konfigurationslagen*. *Acta Cryst.* **A31**, 88–95.
- Koch, E. & Fischer, W. (1985). *Lattice complexes and limiting complexes versus orbit types and non-characteristic orbits: a comparative discussion*. *Acta Cryst.* **A41**, 421–426.
- Koch, E. & Fischer, W. (2006). *Normalizers of space groups, a useful tool in crystal description, comparison and determination*. *Z. Kristallogr.* **221**, 1–14.
- Koch, E. & Müller, U. (1990). *Euklidische Normalisatoren für triklin und monokline Raumgruppen bei spezieller Metrik des Translationengitters*. *Acta Cryst.* **A46**, 826–831.
- Laves, F. (1931). *Ebenenteilung in Wirkungsbereiche*. *Z. Kristallogr.* **76**, 277–284.
- Masse, R., Tordjman, I. & Durif, A. (1976). *Affinement de la structure cristalline du monophosphate d'argent Ag<sub>3</sub>PO<sub>4</sub>. Existence d'une forme haute température*. *Z. Kristallogr.* **144**, 76–81.
- Parthé, E. & Gelato, L. M. (1984). *The standardization of inorganic crystal-structure data*. *Acta Cryst.* **A40**, 169–183.
- Parthé, E. & Gelato, L. M. (1985). *The 'best' unit cell for monoclinic structures consistent with b axis unique and cell choice 1 of International Tables for Crystallography (1983)*. *Acta Cryst.* **A41**, 142–151.
- Schnering, H. G. v. & Hönl, W. (1979). *Zur Chemie und Strukturchemie der Phosphide und Polyphosphide. 20. Darstellung, Struktur und Eigenschaften der Alkalimetallmonophosphide NaP und KP*. *Z. Anorg. Allg. Chem.* **456**, 194–206.
- Schwarzenberger, R. L. E. (1984). *Colour symmetry*. *Bull. London Math. Soc.* **16**, 209–240.
- Sohncke, L. (1879). *Entwicklung einer Theorie der Krystallstruktur*. Leipzig: Teubner.