

15.4. Normalizers of point groups

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Normalizers with respect to the Euclidean or affine group may be defined for any group of isometries (cf. Gubler, 1982*a,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, $m\bar{\infty}$, and of the circle, ∞m , in three-dimensional and two-dimensional space (cf. Galiulin, 1978).

These normalizers are listed in Tables 15.4.1.1 and 15.4.1.2. 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 (∞m ; $m\bar{\infty}$, ∞/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. Section 10.1.2). They give also the relation between the different but equivalent morphological descriptions of a crystal.

Table 15.4.1.1. 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 10.1.4.1.

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

Table 15.4.1.2. 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 10.1.4.2.

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

References

15.1

- 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.
- 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.
- 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.
- Hirshfeld, F. L. (1968). *Symmetry in the generation of trial structures*. *Acta Cryst.* **A24**, 301–311.
- Koch, E. (1984). *A geometrical classification of cubic point configurations*. *Z. Kristallogr.* **166**, 23–52.
- Koch, E. & Fischer, W. (1975). *Automorphismengruppen von Raumgruppen und die Zuordnung von Punktlagen zu Konfigurationen*. *Acta Cryst.* **A31**, 88–95.
- Koch, E. & Müller, U. (1990). *Euklidische Normalisatoren für triklin und monokline Raumgruppen bei spezieller Metrik des Translationengitters*. *Acta Cryst.* **A46**, 826–831.
- 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.

15.2

- 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.
- 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.
- Koch, E. & Müller, U. (1990). *Euklidische Normalisatoren für*

trikline und monokline Raumgruppen bei spezieller Metrik des Translationengitters. *Acta Cryst.* **A46**, 826–831.

- 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.

15.3

- Buttner, R. H. & Maslen, E. N. (1992). *Structural parameters and electron difference density in BaTiO₃*. *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.
- 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. (1985). *Lattice complexes and limiting complexes versus orbit types and non-characteristic orbits: a comparative discussion*. *Acta Cryst.* **A41**, 421–426.
- 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 Ag₃PO₄. Existence d'une forme haute température*. *Z. Kristallogr.* **144**, 76–81.
- Schwarzenberger, R. L. E. (1984). *Colour symmetry*. *Bull. London Math. Soc.* **16**, 209–240.

15.4

- Galiulin, R. V. (1978). *Holoheral varieties of simple forms of crystals*. *Sov. Phys. Crystallogr.* **23**, 635–641.
- 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.