

3. SYMMETRY ASPECTS OF PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

differs in hexagonal and trigonal crystals from the crystallographic coordinate system common in crystallography. Last but not least, a ready-to-use and user-friendly presentation calls for symbols that are explicit and concise.

To meet these requirements, we use in this chapter, in Section 3.1.3 and in the software *GI★KoBo-1* a symbolism in which the orientations of crystallographic elements and operations are expressed by means of suffixes related to a reference Cartesian coordinate system. The relation of this reference Cartesian coordinate system – called a *crystallophysical coordinate system* – to the usual crystallographic coordinate system is a matter of convention. We adhere to the generally accepted rules [see Nye (1985) Appendix B, Sirotnin & Shaskolskaya (1982), Shuvalov (1988), and *IEEE Standards on Piezoelectricity*, 1987].

We list all symbols of crystallographic symmetry operations and a comparison of these symbols with other notations in Tables 3.4.2.5 and 3.4.2.6 and in Figs. 3.4.2.3 and 3.4.2.4.

Now we can present the synoptic Table 3.4.2.7.

3.4.2.4.1. Explanation of Table 3.4.2.7

G: point group expressing the *symmetry of the parent (prototypic) phase*. Subscripts of generators in the group symbol specify their orientation in the Cartesian (rectangular) crystallophysical coordinate system of the group *G* (see Tables 3.4.2.5 and 3.4.2.6, and Figs. 3.4.2.3 and 3.4.2.4).

*F*₁: this point group is a proper subgroup of *G* given in the first column and expresses the *symmetry of the ferroic phase in the first single-domain state S*₁. In accordance with *IT A* (2005), five groups are given in two orientations (bold and normal type). Subscripts of generators in the group symbol specify their orientation in the Cartesian (rectangular) crystallophysical coordinate system of the group *G* (see Tables 3.4.2.5 and 3.4.2.6, and Figs. 3.4.2.3 and 3.4.2.4). In the cubic groups, the direction of the body diagonal is denoted by abbreviated symbols: *p* ≡ [111] (all positive), *q* ≡ [111], *r* ≡ [111], *s* ≡ [111]. In the hexagonal and trigonal groups, axes *x'*, *y'* and *x''*, *y''* of a Cartesian coordinate system are rotated about the *z* axis through 120° and 240°, respectively, from the crystallophysical Cartesian coordinate axes *x* and *y*.

Symmetry groups in parentheses are groups conjugate to *F*₁ under *G* (see Section 3.2.3.2). These are symmetry groups (stabilizers) of some domain states *S*_{*k*} different from *S*₁ (for more details see Section 3.4.2.2.3).

*Γ*_{*η*}: *physically irreducible representation of the group G*. This specifies the transformation properties of the principal tensor parameter of the phase transition in a continuum description and transformation properties of the primary order parameter *η*

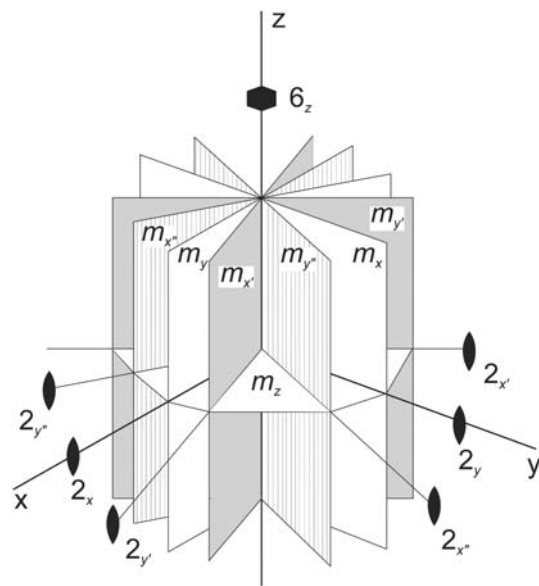


Fig. 3.4.2.4. Oriented symmetry operations of the hexagonal group 6/mmm and of its hexagonal and trigonal subgroups. The coordinate system *x, y, z* corresponds to the Cartesian crystallophysical coordinate system, the axes *x, y, z* of the crystallographic coordinate system are parallel to the twofold rotation axes 2_{*x*}, 2_{*y*} and to the sixfold rotation axis 6_{*z*}. Correlation with other notations is given in Table 3.4.2.6.

of the *equitranslational* phase transitions in the microscopic description. The letters *A, B* signify one-dimensional representations, and letters *E* and *T* two- and three-dimensional irreducible representations, respectively. Two letters *T* indicate that the symmetry descent *G* ⊂ *F*₁ can be accomplished by two non-equivalent three-dimensional irreducible representations (see Table 3.1.3.2). ‘Reducible’ denotes a reducible representation of *G*. In this case, there are always several non-equivalent reducible representations inducing the same descent *G* ⊂ *F*₁ [for more detailed information see the software *GI★KoBo-1* and Kopský (2001)].

Knowledge of *Γ*_{*η*} enables one to determine for all ferroic transitions property tensors and their components that are different in all principal domain states, and, for equitranslational transitions only, microscopic displacements and/or ordering of atoms and molecules that are different in different basic (microscopic) domain states (for details see Section 3.1.3, especially Table 3.1.3.1, and Section 3.1.2).

*N*_{*G*}(*F*₁): the *normalizer of F*₁ in *G* (defined in Section 3.2.3.2.4) determines subgroups conjugate to *F*₁ in *G* and specifies which

Table 3.4.2.6. Symbols of symmetry operations of the point group 6/mmm

Standard: symbols used in Section 3.1.3, in the present chapter and in the software; suffixes (in italic) refer to the Cartesian crystallophysical coordinate system. BC: Bradley & Cracknell (1972). AH: Altmann & Herzog (1994). *IT A*: *IT A* (2005), coordinates (in Sans Serif) are expressed in a crystallographic hexagonal basis. Jones: Jones’ faithful representation symbols express the action of a symmetry operation of a vector (*xyz*) in a crystallographic basis (see e.g. Bradley & Cracknell, 1972).

Standard	BC	AH	<i>IT A</i>	Jones	Standard	BC	AH	<i>IT A</i>	Jones
1 or <i>e</i>	<i>E</i>	<i>E</i>	1	<i>x, y, z</i>	$\bar{1}$ or <i>i</i>	<i>I</i>	<i>I</i>	$\bar{1}$ 0, 0, 0	$\bar{x}, \bar{y}, \bar{z}$
6 _{<i>z</i>}	<i>C</i> ₆ ⁺	<i>C</i> ₆ ⁺	6 ⁺ 0, 0, <i>z</i>	<i>x - y, x, z</i>	$\bar{6}_z$	<i>S</i> ₃ ⁻	<i>S</i> ₃ ⁻	$\bar{6}^+$ 0, 0, <i>z</i>	<i>y - x, \bar{x}, \bar{z}</i>
3 _{<i>z</i>}	<i>C</i> ₃ ⁺	<i>C</i> ₃ ⁺	3 ⁺ 0, 0, <i>z</i>	$\bar{y}, x - y, z$	$\bar{3}_z$	<i>S</i> ₆ ⁻	<i>S</i> ₆ ⁻	$\bar{3}^+$ 0, 0, <i>z</i>	<i>y, y - x, \bar{z}</i>
2 _{<i>z</i>}	<i>C</i> ₂	<i>C</i> ₂	2 0, 0, <i>z</i>	\bar{x}, \bar{y}, z	<i>m</i> _{<i>z</i>}	<i>σ</i> _{<i>h</i>}	<i>σ</i> _{<i>h</i>}	<i>m</i> <i>x, y, 0</i>	<i>x, y, \bar{z}</i>
3 _{<i>z</i>} ²	<i>C</i> ₃ ⁻	<i>C</i> ₃ ⁻	3 ⁻ 0, 0, <i>z</i>	<i>y - x, \bar{x}, z</i>	$\bar{3}_z^5$	<i>S</i> ₆ ⁺	<i>S</i> ₆ ⁺	$\bar{3}^-$ 0, 0, <i>z</i>	<i>x - y, x, \bar{z}</i>
6 _{<i>z</i>} ⁵	<i>C</i> ₆ ⁻	<i>C</i> ₆ ⁻	6 ⁻ 0, 0, <i>z</i>	<i>y, y - x, z</i>	$\bar{6}_z^5$	<i>S</i> ₃ ⁺	<i>S</i> ₃ ⁺	$\bar{6}^-$ 0, 0, <i>z</i>	$\bar{y}, x - y, \bar{z}$
2 _{<i>x</i>}	<i>C</i> ₂₁ ^{''}	<i>C</i> ₂₁ ^{''}	2 <i>x, 0, 0</i>	<i>x - y, \bar{y}, \bar{z}</i>	<i>m</i> _{<i>x</i>}	<i>σ</i> _{<i>v</i>1}	<i>σ</i> _{<i>v</i>1}	<i>m</i> <i>x, 2x, z</i>	<i>y - x, y, z</i>
2 _{<i>x'</i>}	<i>C</i> ₂₂ ^{''}	<i>C</i> ₂₂ ^{''}	2 0, <i>y, 0</i>	$\bar{x}, y - x, \bar{z}$	<i>m</i> _{<i>x'</i>}	<i>σ</i> _{<i>v</i>2}	<i>σ</i> _{<i>v</i>2}	<i>m</i> 2 <i>x, x, z</i>	<i>x, x - y, z</i>
2 _{<i>x''</i>}	<i>C</i> ₂₃ ^{''}	<i>C</i> ₂₃ ^{''}	2 <i>x, x, 0</i>	<i>y, x, \bar{z}</i>	<i>m</i> _{<i>x''</i>}	<i>σ</i> _{<i>v</i>3}	<i>σ</i> _{<i>v</i>3}	<i>m</i> <i>x, \bar{x}, z</i>	\bar{y}, \bar{x}, z
2 _{<i>y</i>}	<i>C</i> ₂₁ [']	<i>C</i> ₂₁ [']	2 <i>x, 2x, 0</i>	<i>y - x, y, \bar{z}</i>	<i>m</i> _{<i>y</i>}	<i>σ</i> _{<i>d</i>1}	<i>σ</i> _{<i>d</i>1}	<i>m</i> <i>x, 0, z</i>	<i>x - y, \bar{y}, z</i>
2 _{<i>y'</i>}	<i>C</i> ₂₂ [']	<i>C</i> ₂₂ [']	2 2 <i>x, x, 0</i>	<i>x, x - y, \bar{z}</i>	<i>m</i> _{<i>y'</i>}	<i>σ</i> _{<i>d</i>2}	<i>σ</i> _{<i>d</i>2}	<i>m</i> 0, <i>y, z</i>	$\bar{x}, y - x, z$
2 _{<i>y''</i>}	<i>C</i> ₂₃ [']	<i>C</i> ₂₃ [']	2 <i>x, $\bar{x}, 0$</i>	$\bar{y}, \bar{x}, \bar{z}$	<i>m</i> _{<i>y''</i>}	<i>σ</i> _{<i>d</i>3}	<i>σ</i> _{<i>d</i>3}	<i>m</i> <i>x, x, z</i>	<i>y, x, z</i>