3.1.3. Equitranslational phase transitions. Property tensors at ferroic phase transitions

By V. Janovec and V. Kopský

In the Landau theory, presented in the preceding Section 3.1.2, symmetry considerations and thermodynamics are closely interwoven. These two aspects can be, at least to some extent, disentangled and some basic symmetry conditions formulated and utilized without explicitly invoking thermodynamics. Statements which follow directly from symmetry are exact but usually do not yield numerical results. These can be obtained by a subsequent thermodynamic or statistical treatment.

The central point of this section is Table 3.1.3.1, which contains results of symmetry analysis for a large class of equitranslational phase transitions and presents data on changes of property tensors at most ferroic phase transitions. Notions and statements relevant to these two applications are explained in Sections 3.1.3.1 and 3.1.3.2, respectively. Table 3.1.3.1 with a detailed explanation is displayed in Section 3.1.3.3. Examples illustrating possible uses of the table are given in Section 3.1.3.4.

3.1.3.1. *Equitranslational phase transitions and their order parameters*

A basic role is played in symmetry considerations by the relation between the space group $\mathcal{G}$ of the high symmetry *parent* or *prototype* phase, the space group $\mathcal{F}$ of the low-symmetry *ferroic* phase and the order parameter η: The low-symmetry group $\mathcal{F}$ consists of all operations of the high-symmetry group $\mathcal{G}$ that leave the order parameter η invariant. By the term *order parameter* we mean the primary order parameter, *i.e.* that set of degrees of freedom whose coefficient of the quadratic invariant changes sign at the phase-transition temperature (see Sections 3.1.2.2.4 and 3.1.2.4.2).

What matters in these considerations is not the physical nature of η but the transformation properties of η, which are expressed by the representation Γ_η of $\mathcal{G}$. The order parameter η with d_η components can be treated as a vector in a d_η-dimensional carrier space V_η of the representation Γ_η, and the low-symmetry group $\mathcal{F}$ comprises all operations of $\mathcal{G}$ that do not change this vector. If Γ_η is a real one-dimensional representation, then the low-symmetry group $\mathcal{F}$ consists of those operations $g \in \mathcal{G}$ for which the matrices $D^{(\eta)}(g)$ [or characters $\chi_\eta(g)$] of the representation Γ_η equal one, $D^{(\eta)}(g) = \chi_\eta(g) = 1$. This condition is satisfied by one half of all operations of $\mathcal{G}$ (index of $\mathcal{F}$ in $\mathcal{G}$ is two) and thus the real one-dimensional representation Γ_η determines the ferroic group $\mathcal{F}$ unambiguously.

A real multidimensional representation Γ_η can induce several low-symmetry groups. A *general vector* of the carrier space V_η of Γ_η is invariant under all operations of a group Ker Γ_η, called the *kernel of representation* Γ_η, which is a normal subgroup of $\mathcal{G}$ comprising all operations $g \in \mathcal{G}$ for which the matrix $D^{(\eta)}(g)$ is the unit matrix. Besides that, *special vectors* of V_η – specified by relations restricting values of order-parameter components (*e.g.* some components of η equal zero, some components are equal *etc.*) – may be invariant under larger groups than the kernel Ker Γ_η. These groups are called *epikernels* of Γ_η (Ascher & Kobayashi, 1977). The kernel and epikernels of Γ_η represent potential symmetries of the ferroic phases associated with the representation Γ_η. Thermodynamic considerations can decide which of these phases is stable at a given temperature and external fields.

Another fundamental result of the Landau theory is that components of the order parameter of all continuous (second-order) and some discontinuous (first-order) phase transitions transform according to an irreducible representation of the space group $\mathcal{G}$ of the high-symmetry phase (see Sections 3.1.2.4.2 and 3.1.2.3). Since the components of the order parameter are real numbers, this condition requires irreducibility over the field of real numbers (so-called *physical irreducibility* or *R-irreducibility*). This means that the matrices $D^{(\eta)}(g)$ of R-irreducible representations (abbreviated *R-ireps*) can contain only real numbers. (Physically irreducible matrix representations are denoted by $D^{(\alpha)}$ instead of the symbol Γ_α used in general considerations.)

As explained in Section 1.2.3 and illustrated by the example of gadolinium molybdate in Section 3.1.2.5, an irreducible representation $\Gamma_{\mathbf{k},m}$ of a space group is specified by a vector $\mathbf{k}$ of the first Brillouin zone, and by an irreducible representation $\tau_m(\mathbf{k})$ of the little group of $\mathbf{k}$, denoted $G(\mathbf{k})$. It turns out that the vector $\mathbf{k}$ determines the change of the translational symmetry at the phase transition (see *e.g* Tolédano & Tolédano, 1987; Izyumov & Syromiatnikov, 1990; Tolédano & Dmitriev, 1996). Thus, unless one restricts the choice of the vector $\mathbf{k}$, one would have an infinite number of phase transitions with different changes of the translational symmetry.

In this section, we restrict ourselves to representations with zero $\mathbf{k}$ vector (this situation is conveniently denoted as the Γ point). Then there is no change of translational symmetry at the transition. In this case, the group $\mathcal{F}$ is called an *equitranslational* or *translationengleiche* (t) *subgroup of* $\mathcal{G}$, and this change of symmetry will be called an *equitranslational symmetry descent* $\mathcal{G} \Downarrow^t \mathcal{F}$. An *equitranslational phase transition* is a transition with an equitranslational symmetry descent $\mathcal{G} \Downarrow^t \mathcal{F}$.

Any ferroic space-group-symmetry descent $\mathcal{G} \Downarrow \mathcal{F}$ uniquely defines the corresponding symmetry descent $G \Downarrow F$, where G and F are the point groups of the space groups $\mathcal{G}$ and $\mathcal{F}$, respectively. Conversely, the equitranslational subgroup $\mathcal{F}$ of a given space group $\mathcal{G}$ is uniquely determined by the point-group symmetry descent $G \Downarrow F$, where G and F are point groups of space groups $\mathcal{G}$ and $\mathcal{F}$, respectively. In other words, a point-group symmetry descent $G \Downarrow F$ defines the set of all equitranslational space-group symmetry descents $\mathcal{G} \Downarrow^t \mathcal{F}$, where $\mathcal{G}$ runs through all space groups with the point group G. All equitranslational space-group symmetry descents $\mathcal{G} \Downarrow^t \mathcal{F}$ are available in the software *GI★KoBo*-1, where more details about the equitranslational subgroups can also be found.

Irreducible and reducible representations of the parent point group G are related in a similar way to irreducible representations with vector $\mathbf{k} = \mathbf{0}$ for all space groups $\mathcal{G}$ with the point group G by a simple process called *engendering* (Jansen & Boon, 1967). The translation subgroup $\mathbf{T}_G$ of $\mathcal{G}$ is a normal subgroup and the point group G is isomorphic to a factor group $\mathcal{G}/\mathbf{T}_G$. This means that to every element $g \in G$ there correspond all elements $\{g|\mathbf{t} + \mathbf{u}_G(g)\}$ of the space group $\mathcal{G}$ with the same linear constituent g, the same non-primitive translation $\mathbf{u}_G(g)$ and any vector $\mathbf{t}$ of the translation group $\mathbf{T}_G$ (see Section 1.2.3.1). If a representation of the point group G is given by matrices $D(g)$, then the corresponding engendered representation of a space group $\mathcal{G}$ with vector $\mathbf{k} = \mathbf{0}$ assigns the same matrix $D(g)$ to all elements $\{g|\mathbf{t} + \mathbf{u}_G(g)\}$ of $\mathcal{G}$.

From this it further follows that a representation Γ_η of a point group G describes transformation properties of the primary order parameter for all equitranslational phase transitions with point-symmetry descent $G \Downarrow F$. This result is utilized in the presentation of Table 3.1.3.1.

3.1.3.2. *Property tensors at ferroic phase transitions. Tensor parameters*

The primary order parameter expresses the 'difference' between the low-symmetry and high-symmetry structures and can be, in a microscopic description, identified with spontaneous displacements of atoms (frozen in soft mode) or with an increase of order of molecular arrangement. To find a microscopic interpretation of order parameters, it is necessary to perform mode analysis (see *e.g.* Rousseau *et al.*, 1981; Aroyo & Perez-Mato, 1998), which takes into account the microscopic structure of the parent phase.

Physical properties of crystals in a continuum description are described by *physical property tensors* (see Section 1.1.1.2), for short *property tensors* [equivalent expressions are *matter tensors* (Nowick, 1995; Wadhawan, 2000) or *material tensors* (Shuvalov, 1988)]. Property tensors are usually expressed in a Cartesian (rectangular) coordinate system [in Russian textbooks called a *crystallophysical system of coordinates* (Sirotin & Shaskolskaya, 1982; Shuvalov, 1988)] which is related to the *crystallographic coordinate system* (*IT* A, 2002) by convention (see *IEEE Standard on Piezoelectricity*, 1987; Sirotin & Shaskolskaya, 1982; Shuvalov, 1988). In what follows, *Cartesian coordinates* will mean coordinates in the crystallophysical system and tensor components will mean components in this coordinate system.

As explained in Section 1.1.4, the number of independent components of property tensors depends on the point-group symmetry of the crystal: the higher this symmetry is, the smaller this number is. Lowering of point-group symmetry at ferroic phase transitions is, therefore, always accompanied by an increased number of independent components of some property tensors. This effect manifests itself by the appearance of *morphic* (Strukov & Levanyuk, 1998) or *spontaneous tensor components*, which are zero in the parent phase and nonzero in the ferroic phase, and/or by symmetry-breaking increments of nonzero components in the ferroic phase that break relations between these tensor components which hold in the parent phase. Thus, for example, the strain tensor has two independent components $u_{11} = u_{22}, u_{33}$ in a tetragonal phase and four independent components $u_{11} \neq u_{22}, u_{33}, u_{12}$ in a monoclinic phase. In a tetragonal-to-monoclinic phase transition there is one morphic component u_{12} and one relation $u_{11} = u_{22}$ is broken by the *symmetry-breaking increment* $\delta u_{11} = -\delta u_{22}$.

Changes of property tensors at a ferroic phase transition can be described in an alternative manner in which no symmetry-breaking increments but only morphic terms appear. As we have seen, the transformation properties of the primary order parameter η are described by a d_η-dimensional R-irreducible matrix representation $D^{(\eta)}$ of the group G. One can form d_η linear combinations of Cartesian tensor components that transform according to the same representation $D^{(\eta)}$. These linear combinations will be called *components of a principal tensor parameter* of the ferroic phase transition with a symmetry descent $G \Downarrow F$. Equivalent designations are *covariant tensor components* (Kopský, 1979*a*) or *symmetry coordinates* (Nowick, 1995) of representation Γ_η of group G. Unlike the primary order parameter of a ferroic phase transition, a principal tensor parameter is not uniquely defined since one can always form further principal tensor parameters from Cartesian components of higher-rank tensors. However, only the principal tensor parameters formed from components of one, or even several, property tensors up to rank four are physically significant.

A principal tensor parameter introduced in this way has the same basic properties as the primary order parameter: it is zero in the parent phase and nonzero in the ferroic phase, and transforms according to the same R-irep $D^{(\eta)}$. However, these two quantities have different physical nature: the primary order parameter of an equitranslational phase transition is a homogeneous microscopic distortion of the parent phase, whereas the principal tensor parameter describes the macroscopic manifestation of this microscopic distortion. Equitranslational phase transitions thus possess the unique property that their primary order parameter can be represented by principal tensor parameters which can be identified and measured by macroscopic techniques.

If the primary order parameter transforms as a vector, the corresponding principal tensor parameter is a dielectric polarization (*spontaneous polarization*) and the equitranslational phase transition is called a *proper ferroelectric phase transition*. Similarly, if the primary order parameter transforms as components of a symmetric second-rank tensor, the corresponding principal tensor parameter is a *spontaneous strain* (or *spontaneous deformation*) and the equitranslational phase transition is called a *proper ferroelastic phase transition.*

A conspicuous feature of equitranslational phase transitions is a steep anomaly (theoretically an infinite singularity for continuous transitions) of the generalized susceptibility associated with the primary order parameter, especially the dielectric susceptibility near a proper ferroelectric transition (see Section 3.1.2.2.5) and the elastic compliance near a proper ferroelastic transition (see *e.g.* Tolédano & Tolédano, 1987; Tolédano & Dmitriev, 1996; Strukov & Levanyuk, 1998).

Any symmetry property of a ferroic phase transition has its pendant in domain structure. Thus it appears that any two ferroic single domain states differ in the values of the principal tensor parameters, *i.e.* principal tensor parameters ensure tensor distinction of any two ferroic domain states. If, in particular, the principal order parameter is polarization, then any two ferroic domain states differ in the direction of spontaneous polarization. Such a ferroic phase is called a *full ferroelectric phase* (Aizu, 1970). In this case, the number of ferroic domain states equals the number of ferroelectric domain states. Similarly, if any two ferroic domain states exhibit different spontaneous strain, then the ferroic phase is a *full ferroelastic phase*. An equivalent condition is an equal number of ferroic and ferroelastic domain states (see Sections 3.4.2.1 and 3.4.2.2).

The principal tensor parameters do not cover all changes of property tensors at the phase transition. Let $D^{(\lambda)}$ be a d_λ-dimensional matrix R-irep of G with an epikernel (or kernel) L which is an intermediate group between F and G, in other words, L is a supergroup of F and a subgroup of G,

$$F \subset L \subset G. \tag{3.1.3.1}$$

This means that a vector λ of the d_λ-dimensional carrier space V_λ of $D^{(\lambda)}$ is invariant under operations of L. The vector λ specifies a *secondary order parameter* of the transition, *i.e.* λ is a morphic quantity, the appearance of which lowers the symmetry from G to L (for more details on secondary order parameters see Tolédano & Tolédano, 1987; Tolédano & Dmitriev, 1996). Intermediate groups (3.1.3.1) can be conveniently traced in lattices of subgroups displayed in Figs. 3.1.3.1 and 3.1.3.2.

One can form linear combinations of Cartesian tensor components that transform according to $D^{(\lambda)}$. These combinations are components of a *secondary tensor parameter* which represents a macroscopic appearance of the secondary order parameter λ.

If a secondary tensor parameter is a spontaneous polarization and no primary order parameter with this property exists, the phase transition is called an *improper ferroelectric phase transition* (Dvořák, 1974; Levanyuk & Sannikov, 1974). Similarly, an *improper ferroelastic phase transition* is specified by existence of a secondary tensor parameter that transforms as components of the symmetric second-rank tensor (spontaneous strain) and by absence of a primary order parameter with this property. Unlike proper ferroelectric and proper ferroelastic phase transitions, which are confined to equitranslational phase transitions, the improper ferroelectric and improper ferroelastic phase transitions appear most often in non-equitranslational phase transitions. Classic examples are an improper ferroelectric phase transition in gadolinium molybdate (see Section 3.1.2.5.2) and an improper ferroelastic phase transition in strontium titanate (see Section 3.1.5.2.3). Examples of equitranslational improper ferroelectric and ferroelastic symmetry descents can be found in Table 3.1.3.2.

Secondary tensor parameters and corresponding susceptibilities exhibit less pronounced changes near the transition than those associated with the primary order parameter (see *e.g.* Tolédano & Tolédano, 1987; Tolédano & Dmitriev, 1996; Strukov & Levanyuk, 1998).

Table 3.1.3.1. *Point-group symmetry descents associated with irreducible representations*

Property tensors that appear in this table: ε enantiomorphism, chirality; P_i dielectric polarization; u_μ strain; g_μ optical activity; $d_{i\mu}$ piezoelectric tensor; $A_{i\mu}$ electrogyration tensor; $\pi_{\mu\nu}$ piezo-optic tensor ($i = 1, 2, 3$; $\mu, \nu = 1, 2, \ldots, 6$). Applications of this table to symmetry analysis of equitranslational phase transitions and to changes of property tensors at ferroic transitions are explained in Section 3.1.3.3.

(*a*) Triclinic parent groups

R-irep Γ_η	Standard variables	Ferroic symmetry F_1		n_F	Principal tensor parameters	Domain states n_f	n_a	n_e
Parent symmetry *G*: 1 C_1								
No ferroic symmetry descent								
Parent symmetry *G*: $\bar{1}$ C_i								
A_u	x_1^-	1	C_1	1	All components of odd parity tensors	2	1	2

(*b*) Monoclinic parent groups

R-irep Γ_η	Standard variables	Ferroic symmetry F_1		n_F	Principal tensor parameters	Domain states n_f	n_a	n_e
Parent symmetry *G*: 2_z C_{2z}								
B	x_3	1	C_1	1	$P_1, P_2; u_4, u_5$	2	2	2
Parent symmetry *G*: m_z C_{sz}								
A''	x_3	1	C_1	1	$\varepsilon; P_3; u_4, u_5$	2	2	2
Parent symmetry *G*: $2_z/m_z$ C_{2hz}								
B_g	x_3^+	$\bar{1}$	C_i	1	u_4, u_5	2	2	0
A_u	x_1^-	2_z	C_{2z}	1	$\varepsilon; P_3$	2	1	2
B_u	x_3^-	m_z	C_{sz}	1	P_1, P_2	2	1	2

(*c*) Orthorhombic parent groups

R-irep Γ_η	Standard variables	Ferroic symmetry F_1		n_F	Principal tensor parameters	Domain states n_f	n_a	n_e
Parent symmetry *G*: $2_x2_y2_z$ D_2								
B_{1g}	x_2	2_z	C_{2z}	1	$P_3; u_6$	2	2	2
B_{3g}	x_3	2_x	C_{2x}	1	$P_1; u_4$	2	2	2
B_{2g}	x_4	2_y	C_{2y}	1	$P_2; u_5$	2	2	2
Parent symmetry *G*: $m_xm_y2_z$ C_{2vz}								
A_2	x_2	2_z	C_{2z}	1	u_6	2	2	1
B_2	x_3	m_x	C_{sx}	1	$P_2; u_4$	2	2	2
B_1	x_4	m_y	C_{sy}	1	$P_1; u_5$	2	2	2
Parent symmetry *G*: $m_xm_ym_z$ D_{2h}								
B_{1g}	x_2^+	$2_z/m_z$	C_{2hz}	1	u_6	2	2	0
B_{3g}	x_3^+	$2_x/m_x$	C_{2hx}	1	u_4	2	2	0
B_{2g}	x_4^+	$2_y/m_y$	C_{2hy}	1	u_5	2	2	0
A_{1u}	x_1^-	$2_x2_y2_z$	D_2	1	$\varepsilon; g_1, g_2, g_3; d_{14}, d_{25}, d_{36}$	2	1	0
B_{1u}	x_2^-	$m_xm_y2_z$	C_{2vz}	1	P_3	2	1	2
B_{3u}	x_3^-	$2_xm_ym_z$	C_{2vx}	1	P_1	2	1	2
B_{2u}	x_4^-	$m_x2_ym_z$	C_{2vy}	1	P_2	2	1	2

(*d*) Tetragonal parent groups

R-irep Γ_η	Standard variables	Ferroic symmetry F_1		n_F	Principal tensor parameters	Domain states n_f	n_a	n_e
Parent symmetry *G*: 4_z C_{4z}								
B	x_3	2_z	C_{2z}	1	$\delta u_1 = -\delta u_2, u_6$	2	2	1
${}^1E \oplus {}^2E$ (Li)	(x_1, y_1)	1	C_1	1	$(P_1, P_2); (u_4, -u_5)$	4	4	4
Parent symmetry *G*: $\bar{4}_z$ S_{4z}								
B	x_3	2_z	C_{2z}	1	$\varepsilon; P_3; \delta u_1 = -\delta u_2, u_6$	2	2	2
${}^1E \oplus {}^2E$	(x_1, y_1)	1	C_1	1	$(P_1, -P_2); (u_4, -u_5)$	4	4	4
Parent symmetry *G*: $4_z/m_z$ C_{4hz}								
B_g	x_3^+	$2_z/m_z$	C_{2hz}	1	$\delta u_1 = -\delta u_2, u_6$	2	2	0
A_u	x_1^-	4_z	C_{4z}	1	$\varepsilon; P_3$	2	1	2
B_u	x_3^-	$\bar{4}_z$	S_{4z}	1	$g_1 = -g_2, g_6; d_{31} = -d_{32}, d_{36}, d_{14} = d_{25}, d_{15} = -d_{24}$	2	1	0
${}^1E_g \oplus {}^2E_g$	(x_1^+, y_1^+)	$\bar{1}$	C_i	1	$(u_4, -u_5)$	4	4	0
${}^1E_u \oplus {}^2E_u$	(x_1^-, y_1^-)	m_z	C_{sz}	1	(P_1, P_2)	4	2	4

Table 3.1.3.1 (*cont.*)

R-irep Γ_η	Standard variables	Ferroic symmetry F_1		n_F	Principal tensor parameters	Domain states n_f	n_a	n_e
Parent symmetry *G*: $\mathbf{4_z 2_x 2_{xy}}$ $\boldsymbol{D_{4z}}$								
A_2	x_2	4_z	C_{4z}	1	P_3	2	1	2
B_1	x_3	$2_x 2_y 2_z$	D_2	1	$\delta u_1 = -\delta u_2$	2	2	0
B_2	x_4	$2_{x\bar{y}} 2_{xy} 2_z$	$\hat{\boldsymbol{D}}_{2z}$	1	u_6	2	2	0
E	$(x_1, 0)$	2_x	C_{2x}	2	P_1; u_4	4	4	4
	(x_1, x_1)	2_{xy}	C_{2xy}	2	$P_1 = P_2$; $u_4 = -u_5$	4	4	4
(Li)	(x_1, y_1)	1	C_1	1	(P_1, P_2); $(u_4, -u_5)$	8	8	8
Parent symmetry *G*: $\mathbf{4_z m_x m_{xy}}$ $\boldsymbol{C_{4vz}}$								
A_2	x_2	4_z	C_{4z}	1	ε; $g_1 = g_2$, g_3; $d_{14} = -d_{25}$	2	1	1
B_1	x_3	$m_x m_y 2_z$	C_{2vz}	1	$\delta u_1 = -\delta u_2$	2	2	1
B_2	x_4	$m_{x\bar{y}} m_{xy} 2_z$	$\hat{\boldsymbol{C}}_{2vz}$	1	u_6	2	2	1
E	$(x_1, 0)$	m_x	C_{sx}	2	P_2; u_4	4	4	4
	(x_1, x_1)	m_{xy}	C_{sxy}	2	$P_2 = -P_1$; $u_4 = -u_5$	4	4	4
	(x_1, y_1)	1	C_1	1	$(P_2, -P_1)$; $(u_4, -u_5)$	8	8	8
Parent symmetry *G*: $\mathbf{\bar{4}_z 2_x m_{xy}}$ $\boldsymbol{D_{2dz}}$								
A_2	x_2	$\bar{4}_z$	S_{4z}	1	g_6; $d_{31} = -d_{32}$, $d_{15} = -d_{24}$	2	1	0
B_1	x_3	$2_x 2_y 2_z$	D_2	1	ε; $\delta u_1 = -\delta u_2$	2	2	0
B_2	x_4	$m_{x\bar{y}} m_{xy} 2_z$	$\hat{\boldsymbol{C}}_{2vz}$	1	P_3; u_6	2	2	2
E	$(x_1, 0)$	2_x	C_{2x}	2	P_1; u_4	4	4	4
	(x_1, x_1)	m_{xy}	C_{sxy}	2	$P_1 = -P_2$; $u_4 = -u_5$	4	4	4
	(x_1, y_1)	1	C_1	1	$(P_1, -P_2)$; $(u_4, -u_5)$	8	8	8
Parent symmetry *G*: $\mathbf{\bar{4}_z m_x 2_{xy}}$ $\boldsymbol{\hat{D}_{2dz}}$								
A_2	x_2	$\bar{4}_z$	S_{4z}	1	$g_1 = -g_2$; d_{36}, $d_{14} = d_{25}$	2	1	0
B_2	x_3	$m_x m_y 2_z$	C_{2vz}	1	P_3; $\delta u_1 = -\delta u_2$	2	2	2
B_1	x_4	$2_{x\bar{y}} 2_{xy} 2_z$	$\hat{D}_{2z}$	1	ε; u_6	2	2	0
E	$(x_1, 0)$	m_x	C_{sx}	2	P_2; u_4	4	4	4
	(x_1, x_1)	2_{xy}	C_{2xy}	2	$P_2 = P_1$; $u_4 = -u_5$	4	4	4
	(x_1, y_1)	1	C_1	1	(P_2, P_1); $(u_4, -u_5)$	8	8	8
Parent symmetry *G*: $\mathbf{4_z/m_z m_x m_{xy}}$ $\boldsymbol{D_{4hz}}$								
A_{2g}	x_2^+	$4_z/m_z$	C_{4hz}	1	$A_{31} = A_{32}$, A_{33}, $A_{15} = A_{24}$	2	1	0
B_{1g}	x_3^+	$m_x m_y m_z$	D_{2h}	1	$\delta u_1 = -\delta u_2$	2	2	0
B_{2g}	x_4^+	$m_{x\bar{y}} m_{xy} m_z$	$\hat{D}_{2hz}$	1	u_6	2	2	0
A_{1u}	x_1^-	$4_z 2_x 2_{xy}$	D_{4z}	1	ε; $g_1 = g_2$, g_3; $d_{14} = -d_{25}$	2	1	0
A_{2u}	x_2^-	$4_z m_x m_{xy}$	C_{4vz}	1	P_3	2	1	2
B_{1u}	x_3^-	$\bar{4}_z 2_x m_{xy}$	D_{2dz}	1	$g_1 = -g_2$; $d_{14} = d_{25}$, d_{36}	2	1	0
B_{2u}	x_4^-	$\bar{4}_z m_x 2_{xy}$	$\hat{D}_{2dz}$	1	g_6; $d_{31} = -d_{32}$, $d_{15} = -d_{24}$	2	1	0
E_g	$(x_1^+, 0)$	$2_x/m_x$	C_{2hx}	2	u_4	4	4	0
	(x_1^+, x_1^+)	$2_{xy}/m_{xy}$	C_{2hxy}	2	$u_4 = -u_5$	4	4	0
	(x_1^+, y_1^+)	$\bar{1}$	C_i	1	$(u_4, -u_5)$	8	8	0
E_u	$(x_1^-, 0)$	$2_x m_y m_z$	C_{2vx}	2	P_1	4	2	4
	(x_1^-, x_1^-)	$m_{x\bar{y}} 2_{xy} m_z$	C_{2vxy}	2	$P_1 = P_2$	4	2	4
	(x_1^-, y_1^-)	m_z	C_{sz}	1	(P_1, P_2)	8	8	8

(*e*) Trigonal parent groups

R-irep Γ_η	Standard variables	Ferroic symmetry F_1		n_F	Principal tensor parameters	Domain states n_f	n_a	n_e
Parent symmetry *G*: $\mathbf{3_z}$ $\boldsymbol{C_3}$								
E	(x_1, y_1)	1	C_1	1	(P_1, P_2) $(u_1 - u_2, -2u_6)$, $(u_4, -u_5)$	3	3	3
(La, Li)					$\delta u_1 = -\delta u_2$			
Parent symmetry *G*: $\mathbf{\bar{3}_z}$ $\boldsymbol{C_{3i}}$								
A_u	x_1^-	3_z	C_3	1	ε; P_3	2	1	2
E_g (La)	(x_1^+, y_1^+)	$\bar{1}$	C_i	1	$(u_1 - u_2, -2u_6)$, $(u_4, -u_5)$ $\delta u_1 = -\delta u_2$	3	3	0
E_u	(x_1^-, y_1^-)	1	C_1	1	(P_1, P_2)	6	3	6
Parent symmetry *G*: $\mathbf{3_z 2_x}$ $\boldsymbol{D_{3x}}$								
A_2	x_2	3_z	C_3	1	P_3	2	1	2
E	$(x_1, 0)$	2_x	C_{2x}	3	P_1; $\delta u_1 = -\delta u_2$, u_4	3	3	3
(La, Li)	(x_1, y_1)	1	C_1	1	(P_1, P_2); $(u_1 - u_2, -2u_6)$, $(u_4, -u_5)$	6	6	6
Parent symmetry *G*: $\mathbf{3_z m_x}$ $\boldsymbol{C_{3vx}}$								
A_2	x_2	3_z	C_3	1	ε; $g_1 = g_2$, g_3; $d_{11} = -d_{12} = -d_{26}$, $d_{14} = -d_{25}$	2	1	1
E	$(x_1, 0)$	m_x	C_{sx}	3	P_2; $\delta u_1 = -\delta u_2$, u_4	3	3	3
(La)	(x_1, y_1)	1	C_1	1	$(P_2, -P_1)$; $(u_1 - u_2, -2u_6)$, $(u_4, -u_5)$	6	6	6

Table 3.1.3.1 (*cont.*)

R-irep Γ_η	Standard variables	Ferroic symmetry F_1		n_F	Principal tensor parameters	Domain states n_f	n_a	n_e
Parent symmetry *G*: $\bar{3}_z m_x$ D_{3dx}								
A_{2g}	x_2^+	$\bar{3}_z$	C_{3i}	1	$A_{22} = -A_{21} = -A_{16}, A_{31} = A_{32}, A_{33}, A_{15} = A_{24}$	2	1	0
A_{1u}	x_1^-	$3_z 2_x$	D_{3x}	1	ε; $g_1 = g_2, g_3$; $d_{11} = -d_{12} = -d_{26}, d_{14} = -d_{25}$	2	1	0
A_{2u}	x_2^-	$3_z m_x$	C_{3vx}	1	P_3	2	1	2
E_g	$(x_1^+, 0)$	$2_x/m_x$	C_{2hx}	3	$\delta u_1 = -\delta u_2, u_4$	3	3	0
(La)	(x_1^+, y_1^+)	$\bar{1}$	C_i	1	$(u_1 - u_2, -2u_6), (u_4, -u_5)$	6	6	0
E_u	$(0, y_1^-)$	m_x	C_{sx}	3	P_2	6	3	6
	$(x_1^-, 0)$	2_x	C_{2x}	3	P_1	6	3	6
	(x_1^-, y_1^-)	1	C_1	1	(P_1, P_2)	12	6	12
Parent symmetry *G*: $3_z 2_y$ D_{3y}								
A_2	x_2	3_z	C_3	1	P_3	2	1	2
E	$(0, y_1)$	2_y	C_{2y}	3	P_2; $\delta u_1 = -\delta u_2, u_5$	3	3	3
(La, Li)	(x_1, y_1)	1	C_1	1	(P_1, P_2); $(2u_6, u_1 - u_2), (u_4, -u_5)$	6	6	6
Parent symmetry *G*: $3_z m_y$ C_{3vy}								
A_2	x_2	3_z	C_3	1	ε; $g_1 = g_2, g_3$; $d_{22} = -d_{21} = -d_{16}, d_{14} = -d_{25}$	2	1	1
E	$(0, y_1)$	m_y	C_{sy}	3	P_1; $\delta u_1 = -\delta u_2, u_5$	3	3	3
(La)	(x_1, y_1)	1	C_1	1	$(P_2, -P_1)$; $(2u_6, u_1 - u_2), (u_4, -u_5)$	6	6	6
Parent symmetry *G*: $\bar{3}_z m_y$ D_{3dy}								
A_{2g}	x_2^+	$\bar{3}_z$	C_{3i}	1	$A_{11} = -A_{12} = -A_{26}, A_{31} = A_{32}, A_{33}, A_{15} = A_{24}$	2	1	0
A_{1u}	x_1^-	$3_z 2_y$	D_{3y}	1	ε; $g_1 = g_2, g_3$; $d_{22} = -d_{21} = -d_{16}, d_{14} = -d_{25}$	2	1	0
A_{2u}	x_2^-	$3_z m_y$	C_{3vy}	1	P_3	2	1	2
E_g	$(0, y_1^+)$	$2_y/m_y$	C_{2hy}	3	$\delta u_1 = -\delta u_2, u_5$	3	3	0
(La)	(x_1^+, y_1^+)	$\bar{1}$	C_i	1	$(2u_6, u_1 - u_2), (u_4, -u_5)$	6	6	0
E_u	$(0, y_1^-)$	2_y	C_{2y}	3	P_2	6	3	6
	$(x_1^-, 0)$	m_y	C_{sy}	3	P_1	6	3	6
	(x_1^-, y_1^-)	1	C_1	1	(P_1, P_2)	12	6	12

(*f*) Hexagonal parent groups

Covariants with standardized labels and conversion equations:

$$g_1^- = g_1 + g_2; \quad g_{2x}^- = g_1 - g_2, \quad g_{2y}^- = 2g_6$$
$$g_1 = \tfrac{1}{2}(g_1^- + g_{2x}^-), \quad g_2 = \tfrac{1}{2}(g_1^- - g_{2x}^-); \quad \delta g_1 = -\delta g_2 = \tfrac{1}{2} g_{2x}^-$$
$$d_1^- = d_{14} - d_{25}; \quad d_{2x,2}^- = d_{14} + d_{25}, \quad d_{2y,2}^- = d_{24} - d_{15}$$
$$d_{2,1}^- = d_{31} + d_{32}; \quad d_{2x,1}^- = 2d_{36}, \quad d_{2y,1}^- = d_{32} - d_{31}$$
$$d_{14} = \tfrac{1}{2}(d_1^- + d_{2x,2}^-), \quad d_{25} = \tfrac{1}{2}(-d_1^- + d_{2x,2}^-); \quad \delta d_{14} = \delta d_{25} = \tfrac{1}{2} d_{2x}^-$$
$$d_{36} = \tfrac{1}{2} d_{2x,1}^-, \quad d_{31} = \tfrac{1}{2}(d_{2,1}^- - d_{2y,1}^-); \quad d_{32} = \tfrac{1}{2}(d_{2,1}^- + d_{2y,1}^-).$$

R-irep Γ_η	Standard variables	Ferroic symmetry F_1		n_F	Principal tensor parameters	Domain states n_f	n_a	n_e
Parent symmetry *G*: 6_z C_6								
B	x_3	3_z	C_3	1	$d_{11} = -d_{12} = -d_{26}, d_{22} = -d_{21} = -d_{16}$	2	1	1
E_2	(x_2, y_2)	2_z	C_{2z}	1	$(u_1 - u_2, 2u_6)$ $\delta u_1 = -\delta u_2$	3	3	1
(La, Li)								
E_1	(x_1, y_1)	1	C_1	1	(P_1, P_2)	6	6	6
(Li)					$(u_4, -u_5)$			
Parent symmetry *G*: $\bar{6}_z$ C_{3h}								
A''	x_3	3_z	C_3	1	ε; P_3	2	1	2
E'	(x_2, y_2)	m_z	C_{sz}	1	(P_2, P_1)	3	3	3
(La)					$(u_1 - u_2, 2u_6)$ $\delta u_1 = -\delta u_2$			
E''	(x_1, y_1)	1	C_1	1	$(u_4, -u_5)$	6	6	6
Parent symmetry *G*: $6_z/m_z$ C_{6h}								
B_g	x_3^+	$\bar{3}_z$	C_{3i}	1	$A_{11} = -A_{12} = -A_{26}, A_{22} = -A_{21} = -A_{16}$	2	1	0
A_u	x_1^-	6_z	C_6	1	ε; P_3	2	1	2
B_u	x_3^-	$\bar{6}_z$	C_{3h}	1	$d_{11} = -d_{12} = -d_{26}, d_{22} = -d_{21} = -d_{16}$	2	1	0
E_{2g}	(x_2^+, y_2^+)	$2_z/m_z$	C_{2hz}	1	$(u_1 - u_2, 2u_6)$ $\delta u_1 = -\delta u_2$	3	3	0
(La)								
E_{1g}	(x_1^+, y_1^+)	$\bar{1}$	C_i	1	$(u_4, -u_5)$	6	6	0
E_{2u}	(x_2^-, y_2^-)	2_z	C_{2z}	1	$(g_1 - g_2, 2g_6)$ $g_1 = -g_2, g_6$	6	3	2
					$(2d_{36}, d_{32} - d_{31})$ $d_{32} = -d_{31}, d_{36}$			
					$(d_{14} + d_{25}, d_{24} - d_{15})$ $d_{14} = d_{25}, d_{24} = -d_{15}$			
E_{1u}	(x_1^-, y_1^-)	m_z	C_{sz}	1	(P_1, P_2)	6	3	6

Table 3.1.3.1 (*cont.*)

R-irep Γ_η	Standard variables	Ferroic symmetry F_1		n_F	Principal tensor parameters	Domain states n_f	n_a	n_e
Parent symmetry G:		$\mathbf{6_z 2_x 2_y}$	$\boldsymbol{D_6}$					
A_2	x_2	6_z	C_6	1	P_3	2	1	2
B_1	x_3	$3_z 2_x$	D_{3x}	1	$d_{11} = -d_{12} = -d_{26}$	2	1	0
B_2	x_4	$3_z 2_y$	D_{3y}	1	$d_{22} = -d_{21} = -d_{16}$	2	1	0
E_2	$(x_2, 0)$	$2_x 2_y 2_z$	D_2	3	$\delta u_1 = -\delta u_2$	3	3	0
(La, Li)	(x_2, y_2)	2_z	C_{2z}	1	$(u_1 - u_2, 2u_6)$	6	6	2
E_1	$(x_1, 0)$	2_x	C_{2x}	3	P_1; u_4	6	6	6
	$(0, y_1)$	2_y	C_{2y}	3	P_2; u_5	6	6	6
(Li)	(x_1, y_1)	1	C_1	1	(P_1, P_2); $(u_4, -u_5)$	12	12	12
Parent symmetry G:		$\mathbf{6_z m_x m_y}$	$\boldsymbol{C_{6v}}$					
A_2	x_2	6_z	C_6	1	ε; $g_1 = g_2, g_3$; $d_{14} = -d_{25}$	2	1	1
B_2	x_3	$3_z m_x$	C_{3vx}	1	$d_{22} = -d_{21} = -d_{16}$	2	1	1
B_1	x_4	$3_z m_y$	C_{3vy}	1	$d_{11} = -d_{12} = -d_{26}$	2	1	1
E_2	$(x_2, 0)$	$m_x m_y 2_z$	C_{2vz}	3	$\delta u_1 = -\delta u_2$	3	3	1
(La)	(x_2, y_2)	2_z	C_{2z}	1	$(u_1 - u_2, 2u_6)$	6	6	1
E_1	$(x_1, 0)$	m_x	C_{sx}	3	P_2; u_4	6	6	6
	$(0, y_1)$	m_y	C_{sy}	3	P_1; u_5	6	6	6
	(x_1, y_1)	1	C_1	1	$(P_2, -P_1)$; $(u_4, -u_5)$	12	12	12
Parent symmetry G:		$\mathbf{\bar{6}_z 2_x m_y}$	$\boldsymbol{D_{3h}}$					
A_2'	x_2	$\bar{6}_z$	C_{3h}	1	$d_{22} = -d_{21} = -d_{16}$	2	1	0
A_1''	x_3	$3_z 2_x$	D_{3x}	1	ε; $g_1 = g_2, g_3$; $d_{14} = -d_{25}$	2	1	0
A_2''	x_4	$3_z m_y$	C_{3vy}	1	P_3	2	1	2
E'	$(x_2, 0)$	$2_x m_y m_z$	C_{2vx}	3	P_1; $\delta u_1 = -\delta u_2$	3	3	3
(La)	(x_2, y_2)	m_z	C_{sz}	1	$(P_1, -P_2)$; $(u_1 - u_2, 2u_6)$	6	6	6
E''	$(x_1, 0)$	2_x	C_{2x}	3	u_4	6	6	3
	$(0, y_1)$	m_y	C_{sy}	3	u_5	6	6	6
	(x_1, y_1)	1	C_1	1	$(u_4, -u_5)$	12	12	12
Parent symmetry G:		$\mathbf{\bar{6}_z m_x 2_y}$	$\boldsymbol{\hat{D}_{3h}}$					
A_2'	x_2	$\bar{6}_z$	C_{3h}	1	$d_{11} = -d_{12} = -d_{26}$	2	1	0
A_2''	x_3	$3_z m_x$	C_{3vx}	1	P_3	2	1	2
A_1'	x_4	$3_z 2_y$	D_{3y}	1	ε; $g_1 = g_2, g_3$; $d_{14} = -d_{25}$	2	1	0
E'	$(x_2, 0)$	$m_x 2_y m_z$	C_{2vy}	3	P_2; $\delta u_1 = -\delta u_2$	3	3	3
(La)	(x_2, y_2)	m_z	C_{sz}	1	(P_2, P_1); $(u_1 - u_2, 2u_6)$	6	6	6
E''	$(x_1, 0)$	m_x	C_{sx}	3	u_4	6	6	6
	$(0, y_1)$	2_y	C_{2y}	3	u_5	6	6	3
	(x_1, y_1)	1	C_1	1	$(u_4, -u_5)$	12	12	12
Parent symmetry G:		$\mathbf{6_z/m_z m_x m_y}$	$\boldsymbol{D_{6h}}$					
A_{2g}	x_2^+	$6_z/m_z$	C_{6h}	1	$A_{31} = A_{32}, A_{33}, A_{15} = A_{24}$	2	1	0
B_{1g}	x_3^+	$\bar{3}_z m_x$	D_{3dx}	1	$A_{11} = -A_{12} = -A_{26}$	2	1	0
B_{2g}	x_4^+	$\bar{3}_z m_y$	D_{3dy}	1	$A_{22} = -A_{21} = -A_{16}$	2	1	0
A_{1u}	x_1^-	$6_z 2_x 2_y$	D_6	1	ε; $g_1 = g_2, g_3$; $d_{14} = -d_{25}$	2	1	0
A_{2u}	x_2^-	$6_z m_x m_y$	C_{6v}	1	P_3	2	1	2
B_{1u}	x_3^-	$\bar{6}_z 2_x m_y$	D_{3h}	1	$d_{11} = -d_{12} = -d_{26}$	2	1	0
B_{2u}	x_4^-	$\bar{6}_z m_x 2_y$	$\hat{D}_{3h}$	1	$d_{22} = -d_{21} = -d_{16}$	2	1	0
E_{2g}	$(x_2^+, 0)$	$m_x m_y m_z$	D_{2h}	3	$\delta u_1 = -\delta u_2$	3	3	0
(La)	(x_2^+, y_2^+)	$2_z/m_z$	C_{2hz}	1	$(u_1 - u_2, 2u_6)$	6	6	0
E_{1g}	$(x_1^+, 0)$	$2_x/m_x$	C_{2hx}	3	u_4	6	6	0
	$(0, y_1^+)$	$2_y/m_y$	C_{2hy}	3	u_5	6	6	0
	(x_1^+, y_1^+)	$\bar{1}$	C_i	1	$(u_4, -u_5)$	12	12	0
E_{1u}	$(x_1^-, 0)$	$2_x m_y m_z$	C_{2vx}	3	P_1	6	3	6
	$(0, y_1^-)$	$m_x 2_y m_z$	C_{2vy}	3	P_2	6	3	6
	(x_1^-, y_1^-)	m_z	C_{sz}	1	(P_1, P_2)	12	6	12
E_{2u}	$(x_2^-, 0)$	$2_x 2_y 2_z$	D_2	3	$\delta g_1 = -\delta g_2$; d_{36}, $\delta d_{14} = \delta d_{25}$	6	3	0
	$(0, y_2^-)$	$m_x m_y 2_z$	C_{2vz}	3	g_6: $d_{32} = -d_{31}$, $d_{24} = -d_{15}$	6	3	2
	(x_2^-, y_2^-)	2_z	C_{2z}	1	$(g_1 - g_2, 2g_6)$; $(2d_{36}, d_{32} - d_{31})$, $(d_{14} + d_{25}, d_{24} - d_{15})$	12	6	2

In tensor distinction of domains, the secondary tensor parameters play a secondary role in a sense that some but not all ferroic domain states exhibit different values of the secondary tensor parameters. This property forms a basis for the concept of partial ferroic phases (Aizu, 1970): A ferroic phase is a *partial ferroelectric (ferroelastic)* one if some but not all domain states differ in spontaneous polarization (spontaneous strain). A non-ferroelectric phase denotes a ferroic phase which is either non-polar or which possesses a unique polar direction available already in the parent phase. A non-ferroelastic phase exhibits no spontaneous strain.

3.1.3.3. *Tables of equitranslational phase transitions associated with irreducible representations*

The first systematic symmetry analysis of Landau-type phase transitions was performed by Indenbom (1960), who found all equitranslational phase transitions that can be accomplished

Table 3.1.3.1 (*cont.*)

(*g*) Cubic parent groups

Covariants with standardized labels and conversion equations:

$$u_{3x} = u_{3x}^{+} = u_3 - a(u_1 + u_2); \quad u_{3y} = u_{3y}^{+} = b(u_1 - u_2)$$
$$\delta u_1 = -\tfrac{1}{3}u_{3x}^{+} + \tfrac{1}{\sqrt{3}}u_{3y}^{+}; \quad \delta u_2 = -\tfrac{1}{3}u_{3x}^{+} - \tfrac{1}{\sqrt{3}}u_{3y}^{+}; \quad \delta u_3 = \tfrac{2}{3}u_{3x}^{+}$$
$$g_1^{-} = g_1 + g_2 + g_3; \quad g_{3x}^{-} = g_3 - a(g_1 + g_2); \quad g_{3y}^{-} = b(g_1 - g_2)$$
$$g_1 = \tfrac{1}{3}g_1^{-} - \tfrac{1}{3}g_{3x}^{-} + \tfrac{1}{\sqrt{3}}g_{3y}^{-}; \quad g_2 = \tfrac{1}{3}g_1^{-} - \tfrac{1}{3}g_{3x}^{-} - \tfrac{1}{\sqrt{3}}g_{3y}^{-}; \quad g_3 = \tfrac{1}{3}g_1^{-} + \tfrac{2}{3}g_{3x}^{-}$$
$$d_1^{-} = d_{14} + d_{25} + d_{36}; \quad d_{3x}^{-} = b(d_{14} - d_{25}), \quad d_{3y}^{-} = a(d_{14} + d_{25}) - d_{36}$$
$$d_{14} = \tfrac{1}{3}d_1^{-} + \tfrac{1}{\sqrt{3}}d_{3x}^{-} + \tfrac{1}{3}d_{3y}^{-}; \quad d_{25} = \tfrac{1}{3}d_1^{-} - \tfrac{1}{\sqrt{3}}d_{3x}^{-} + \tfrac{1}{3}d_{3y}^{-}; \quad d_{36} = \tfrac{1}{3}d_1^{-} - \tfrac{2}{3}d_{3y}^{-}$$
$$d_{1x} = d_{13} - d_{12}; \quad d_{1y} = d_{21} - d_{23}; \quad d_{1z} = d_{32} - d_{31}$$
$$d_{2x} = d_{13} + d_{12}; \quad d_{2y} = d_{21} + d_{23}; \quad d_{2z} = d_{32} + d_{31}$$
$$d_{13} = \tfrac{1}{2}(d_{1x} + d_{2x}); \quad d_{21} = \tfrac{1}{2}(d_{1y} + d_{2y}); \quad d_{32} = \tfrac{1}{2}(d_{1z} + d_{2z})$$
$$d_{12} = \tfrac{1}{2}(d_{2x} - d_{1x}); \quad d_{23} = \tfrac{1}{2}(d_{2y} - d_{1y}); \quad d_{31} = \tfrac{1}{2}(d_{2z} - d_{1z})$$

$a = \frac{1}{2}$, $b = \frac{\sqrt{3}}{2}$, $\pi^{a}_{\mu\nu} = (\pi_{\mu\nu} - \pi_{\nu\mu})$, $\mu = 1, 2, \ldots, 6$, $\nu = 1, 2, \ldots, 6$.

R-irep Γ_η	Standard variables	Ferroic symmetry F_1		n_F	Principal tensor parameters	Domain states n_f	n_a	n_e
Parent symmetry *G*: 23 *T*								
E (La)	(x_3, y_3)	$2_x2_y2_z$	D_2	1	$[u_3 - a(u_1+u_2), b(u_1-u_2)]$ $\delta u_1 + \delta u_2 + \delta u_3 = 0$	3	3	0
T	$(0, 0, z_1)$	2_z	C_{2z}	3	P_3; u_6	6	6	6
	(x_1, x_1, x_1)	3_p	C_{3p}	4	$P_1 = P_2 = P_3$; $u_4 = u_5 = u_6$	4	4	4
(La, Li)	(x_1, y_1, z_1)	1	C_1	1	(P_1, P_2, P_3); (u_4, u_5, u_6)	12	12	12
Parent symmetry *G*: $m\bar{3}$ T_h								
A_u	x_1^{-}	23	T	1	ε; $g_1 = g_2 = g_3$; $d_{14} = d_{25} = d_{36}$	2	1	0
E_g (La)	(x_3^{+}, y_3^{+})	$m_xm_ym_z$	D_{2h}	1	$[u_3 - a(u_1+u_2), b(u_1-u_2)]$ $\delta u_1 + \delta u_2 + \delta u_3 = 0$	3	3	0
E_u	(x_3^{-}, y_3^{-})	$2_x2_y2_z$	D_2	1	$[g_3 - a(g_1+g_2), b(g_1-g_2)]$ $\delta g_1 + \delta g_2 + \delta g_3 = 0$ $[b(d_{14}-d_{25}), a(d_{14}+d_{25}) - d_{36}]$ $\delta d_{14} + \delta d_{25} + \delta d_{36} = 0$	6	3	0
T_g	$(0, 0, z_1^{+})$	$2_z/m_z$	C_{2hz}	3	u_6	6	6	0
	$(x_1^{+}, x_1^{+}, x_1^{+})$	$\bar{3}_p$	C_{3ip}	4	$u_4 = u_5 = u_6$	4	4	0
(La)	$(x_1^{+}, y_1^{+}, z_1^{+})$	$\bar{1}$	C_i	1	(u_4, u_5, u_6)	12	12	0
T_u	$(0, 0, z_1^{-})$	$m_xm_y2_z$	C_{2vz}	3	P_3	6	3	6
	$(x_1^{-}, x_1^{-}, x_1^{-})$	3_p	C_{3p}	4	$P_1 = P_2 = P_3$	8	4	8
	$(x_1^{-}, y_1^{-}, z_1^{-})$	1	C_1	1	(P_1, P_2, P_3)	24	12	24
Parent symmetry *G*: 432 *O*								
A_2	x_2	23	T	1	$d_{14} = d_{25} = d_{36}$	2	1	0
E	$(x_3, 0)$	$4_z2_x2_{xy}$	D_{4z}	3	$\delta u_1 = \delta u_2 = -\frac{1}{2}\delta u_3$	3	3	0
(La)	(x_3, y_3)	$2_x2_y2_z$	D_2	1	$[u_3 - a(u_1+u_2), b(u_1-u_2)]$ $\delta u_1 + \delta u_2 + \delta u_3 = 0$	6	6	0
T_1	$(0, 0, z_1)$	4_z	C_{4z}	3	P_3	6	3	6
	$(x_1, x_1, 0)$	2_{xy}	C_{2xy}	6	$P_1 = P_2$	12	12	12
	(x_1, x_1, x_1)	3_p	C_{3p}	4	$P_1 = P_2 = P_3$	8	4	8
(Li)	(x_1, y_1, z_1)	1	C_1	1	(P_1, P_2, P_3)	24	24	24
T_2	$(0, 0, z_2)$	$2_{x\bar{y}}2_{xy}2_z$	$\hat{D}_{2z}$	3	u_6	6	6	0
	$(x_2, -x_2, z_2)$	2_{xy}	C_{2xy}	6	$u_4 = -u_5$, u_6	12	12	12
	(x_2, x_2, x_2)	$3_p2_{x\bar{y}}$	D_{3p}	4	$u_4 = u_5 = u_6$	4	4	0
(La, Li)	(x_2, y_2, z_2)	1	C_1	1	(u_4, u_5, u_6)	24	24	24

continuously. A table of all crystallographic point groups G along with all their physically irreducible representations, corresponding ferroic point groups F and related data has been compiled by Janovec *et al.* (1975). These data are presented in an improved form in Table 3.1.3.1 together with corresponding principal tensor parameters and numbers of ferroic, ferroelectric and ferroelastic domain states. This table facilitates solving of the following typical problems:

(1) *Inverse Landau problem* (Ascher & Kobayashi, 1977) of equitranslational phase transitions: For a given equitranslational symmetry descent $\mathcal{G} \Downarrow^{t} \mathcal{F}$ (determined for example from diffraction experiments), find the representation Γ_η of $\mathcal{G}$ that specifies the transformation properties of the primary order parameter. Solution: In Table 3.1.3.1, one finds a physically irreducible representation Γ_η of the point group G of $\mathcal{G}$ with epikernel F (point group of $\mathcal{F}$). For some symmetry descents from cubic point groups $G = 432$, $\bar{4}3m$ and $m\bar{3}m$, the inverse Landau problem has two solutions, which are given in Table 3.1.3.2.

If for a given symmetry descent $\mathcal{G} \Downarrow^{t} \mathcal{F}$ no appropriate *R*-irep exists in Table 3.1.3.1, then the primary order parameter η transforms according to a reducible representation of G. These transitions are always discontinuous and can be accomplished with several reducible representations. Some symmetry descents can be associated with an irreducible representation and with several reducible representations. All these transitions are treated in the software *GI★KoBo*-1 and in Kopský (2001). All point-group symmetry descents are listed in Table 3.4.2.7 and can be traced in lattices of subgroups (see Figs. 3.1.3.1 and 3.1.3.2).

Table 3.1.3.1 (*cont.*)

R-irep Γ_η	Standard variables	Ferroic symmetry F_1		n_F	Principal tensor parameters	Domain states n_f	n_a	n_e
Parent symmetry *G*: $\bar{4}3m$ T_d								
A_2	x_2	23	T	1	ε; $g_1 = g_2 = g_3$ $A_{14} = A_{25} = A_{36}$; $\pi^a_{23} = \pi^a_{31} = \pi^a_{12}$	2	1	0
E	$(x_3, 0)$	$\bar{4}_z 2_x m_{xy}$	D_{2dz}	3	$\delta u_1 = \delta u_2 = -\frac{1}{2}\delta u_3$	3	3	0
(La)	(x_3, y_3)	$2_x 2_y 2_z$	D_2	1	$[u_3 - a(u_1 + u_2), b(u_1 - u_2)]$ $\delta u_1 + \delta u_2 + \delta u_3 = 0$	6	6	0
T_1	$(0, 0, z_1)$	$\bar{4}_z$	S_{4z}	3	g_6; $d_{32} = -d_{31}$, $d_{24} = -d_{15}$	6	3	0
	$(x_1, x_1, 0)$	m_{xy}	C_{sxy}	6	$g_4 = g_5$ $d_{13} = -d_{23}$, $d_{12} = -d_{21}$ $d_{35} = -d_{34}$, $d_{26} = -d_{16}$	12	12	12
	(x_1, x_1, x_1)	3_p	C_{3p}	4	$g_4 = g_5 = g_6$ $d_{13} = d_{21} = d_{32}$, $d_{12} = d_{23} = d_{31}$ $d_{35} = d_{16} = d_{24}$, $d_{26} = d_{34} = d_{15}$	8	4	4
	(x_1, y_1, z_1)	1	C_1	1	(g_4, g_5, g_6) $(d_{13} - d_{12}, d_{21} - d_{23}, d_{32} - d_{31})$ $(d_{35} - d_{26}, d_{16} - d_{34}, d_{24} - d_{15})$	24	24	24
T_2	$(0, 0, z_2)$	$m_{x\bar{y}} m_{xy} 2_z$	$\hat{C}_{2vz}$	3	P_3; u_6	6	6	6
	$(x_2, -x_2, z_2)$	m_{xy}	C_{sxy}	6	$P_1 = -P_2$, P_3; $u_4 = -u_5$, u_6	12	12	12
	(x_2, x_2, x_2)	$3_p m_{x\bar{y}}$	C_{3vp}	4	$P_1 = P_2 = P_3$; $u_4 = u_5 = u_6$	4	4	4
(La)	(x_2, y_2, z_2)	1	C_1	1	(P_1, P_2, P_3); (u_4, u_5, u_6)	24	24	24
Parent symmetry *G*: $m\bar{3}m$ O_h								
A_{2g}	x_2^+	$m\bar{3}$	T_h	1	$A_{14} = A_{25} = A_{36}$; $\pi^a_{23} = \pi^a_{31} = \pi^a_{12}$	2	1	0
A_{1u}	x_1^-	432	O	1	ε; $g_1 = g_2 = g_3$;	2	1	0
A_{2u}	x_2^-	$\bar{4}3m$	T_d	1	$d_{14} = d_{25} = d_{36}$	2	1	0
E_g	$(x_3^+, 0)$	$4_z / m_z m_x m_{xy}$	D_{4hz}	3	δu_3	3	3	0
(La)	(x_3^+, y_3^+)	$m_x m_y m_z$	D_{2h}	1	$[\delta u_3 - a(\delta u_1 + \delta u_2), b(\delta u_1 - \delta u_2)]$	6	6	0
E_u	$(x_3^-, 0)$	$4_z 2_x 2_{xy}$	D_{4z}	3	$g_1 = g_2, g_3$; $d_{14} = -d_{25}$	12	3	0
	$(0, y_3^-)$	$\bar{4}_z 2_x m_{xy}$	D_{2dz}	3	$g_1 = -g_2$; $d_{14} = d_{25} = d_{36}$	6	3	0
	(x_3^-, y_3^-)	$2_x 2_y 2_z$	D_2	1	$[g_3 - a(g_1 + g_2), b(g_1 - g_2)]$ $[b(d_{14} - d_{25}), a(d_{14} + d_{25}) - d_{36}]$	12	6	0
T_{1g}	$(0, 0, z_1^+)$	$4_z / m_z$	C_{4hz}	3	$A_{33}, A_{32} = A_{31}, A_{24} = A_{15}, A_{14} = -A_{25}$	6	3	0
	$(x_1^+, x_1^+, 0)$	$2_{xy} / m_{xy}$	C_{2hxy}	6	$A_{11} = A_{22}$, $A_{13} = A_{23}$, $A_{12} = A_{21}$ $A_{35} = A_{34}$, $A_{26} = A_{16}$	12	12	0
	(x_1^+, x_1^+, x_1^+)	$\bar{3}_p$	C_{3ip}	4	$A_{11} = A_{22} = A_{33}$ $A_{13} = A_{21} = A_{32}$, $A_{12} = A_{32} = A_{31}$ $A_{35} = A_{16} = A_{24}$, $A_{26} = A_{34} = A_{15}$	8	4	0
	(x_1^+, y_1^+, z_1^+)	$\bar{1}$	C_i	1	(A_{11}, A_{22}, A_{33}) $(A_{13} + A_{12}, A_{21} + A_{23}, A_{32} + A_{31})$ $(A_{35} + A_{26}, A_{16} + A_{34}, A_{24} + A_{15})$	24	24	0
T_{2g}	$(0, 0, z_2^+)$	$m_{x\bar{y}} m_{xy} m_z$	$\hat{D}_{2hz}$	3	u_6	6	6	0
	$(x_2^+, -x_2^+, z_2^+)$	$2_{xy} / m_{xy}$	C_{2hxy}	6	$u_4 = -u_5$, u_6	24	12	12
	(x_2^+, x_2^+, x_2^+)	$\bar{3}_p m_{x\bar{y}}$	D_{3dp}	4	$u_4 = u_5 = u_6$	4	4	0
(La)	(x_2^+, y_2^+, z_2^+)	$\bar{1}$	C_i	1	(u_4, u_5, u_6)	24	24	0
T_{1u}	$(0, 0, z_1^-)$	$4_z m_x m_{xy}$	C_{4vz}	3	P_3	6	3	6
	$(x_1^-, y_1^-, 0)$	m_z	C_{sz}	3	P_1,P_2	24	12	24
	$(x_1^-, x_1^-, 0)$	$m_{x\bar{y}} 2_{xy} m_z$	$\hat{C}_{2vxy}$	6	$P_1 = P_2$	12	6	12
	$(x_1^-, -x_1^-, z_1^-)$	m_{xy}	C_{sxy}	6	$P_1 = -P_2$, P_3	24	12	24
	(x_1^-, x_1^-, x_1^-)	$3_p m_{x\bar{y}}$	C_{3vp}	4	$P_1 = P_2 = P_3$	8	4	8
	(x_1^-, y_1^-, z_1^-)	1	C_1	1	(P_1, P_2, P_3)	48	24	48
T_{2u}	$(0, 0, z_2^-)$	$\bar{4}_z m_x 2_{xy}$	$\hat{D}_{2dz}$	3	g_6; $d_{32} = -d_{31}$, $d_{24} = -d_{15}$	6	3	0
	$(x_2^-, y_2^-, 0)$	m_z	C_{sz}	3	g_4, g_5; $d_{13}, d_{12}, d_{21}, d_{23}$ $d_{35}, d_{26}, d_{16}, d_{34}$	24	12	24
	$(x_2^-, -x_2^-, 0)$	$m_{x\bar{y}} 2_{xy} m_z$	$\hat{C}_{2vxy}$	6	$g_4 = -g_5$; $d_{13} = d_{23}$, $d_{21} = d_{21}$ $d_{35} = d_{34}$, $d_{16} = d_{26}$	12	6	12
	$(x_2^-, -x_2^-, z_2^-)$	2_{xy}	C_{2xy}	6	$g_4 = -g_5$, g_6; $d_{13} = d_{23}$, $d_{21} = d_{21}$ $d_{35} = d_{34}$, $d_{16} = d_{26}$ $d_{32} = -d_{31}$, $d_{24} = -d_{15}$	24	12	12
	(x_2^-, x_2^-, x_2^-)	$3_p 2_{x\bar{y}}$	D_{3p}	4	$g_4 = g_5 = g_6$; $d_{13} = -d_{12} = d_{21} = -d_{23} = d_{32} - d_{31}$ $d_{35} = -d_{26} = d_{16} = -d_{34} = d_{24} = -d_{15}$	8	4	0
	(x_2^-, y_2^-, z_2^-)	1	C_1	1	(g_4, g_5, g_6) $(d_{13} - d_{12}, d_{21} - d_{23}, d_{32} - d_{31})$ $(d_{35} - d_{26}, d_{16} - d_{34}, d_{24} - d_{15})$	48	24	48

The solution of the inverse Landau problem – *i.e.* the identification of the representation Γ_η relevant to symmetry descent $G \Downarrow F$ – enables one to determine the corresponding nomal mode (so-called soft mode) of the transition (see *e.g.* Rousseau *et al.*, 1981). We note that this step requires additional knowledge of the crystal structure, whereas other conclusions of the analysis hold for *any* crystal structure with a given symmetry descent $G \Downarrow F$. Normal-mode determination reveals the dynamic microscopic nature of the instability of the crystal lattice which leads to the phase transition (for more details and examples, see Section 3.1.5).

The representation Γ_η further determines the principal tensor parameters associated with the primary order parameter η. If one of them is a vector (polarization) the soft mode is infrared-active in the parent phase; if it is a symmetric second-rank tensor (spontaneous strain), the soft mode is Raman active in this phase. Furthermore, the *R*-irep Γ_η determines the polynomial in components of η in the Landau free energy (basic invariant polynomials, called *integrity bases*, are available in the software *GI⋆KoBo*-1 and in Kopský, 2001) and allows one to decide whether the necessary conditions of continuity of the transition (so-called Landau and Lifshitz conditions) are fulfilled.

(2) *Direct Landau problem of equitranslational phase transitions*: For a given space group $\mathcal{G}$ of the parent phase and the *R*-irep Γ_η (specifying the transformation properties of the primary order parameter η), find the corresponding equitranslational space group $\mathcal{F}$ of the ferroic phase. To solve this task, one first finds in Table 3.1.3.1 the point group F that corresponds to point group G of space group $\mathcal{G}$ and to the given *R*-irep Γ_η. The point-group symmetry descent $G \Downarrow F$ thus obtained specifies uniquely the equitranslational subgroup $\mathcal{F}$ of $\mathcal{G}$ that can be found in the lattices of equitranslational subgroups of space groups available in the software *GI⋆KoBo*-1 (see Section 3.1.6).

(3) *Secondary tensor parameters of an equitranslational phase transition* $\mathcal{G} \Downarrow^t \mathcal{F}$. These parameters are specified by the representation Γ_λ of G associated with a symmetry descent $\Gamma \Downarrow L$, where L is an intermediate group [see equation (3.1.3.1)]. In other words, the secondary tensor parameters of the transition $G \Downarrow F$ are identical with principal tensor parameters of the transition $G \Downarrow L$. To each intermediate group L there corresponds a set of secondary tensor parameters. All intermediate subgroups of a symmetry descent $G \Downarrow F$ can be deduced from lattices of subgroups in Figs. 3.1.3.1 and 3.1.3.2.

The representation Γ_λ specifies transformation properties of the secondary tensor parameter λ and thus determines *e.g* its infrared and Raman activity in the parent phase and enables one to make a mode analysis. Representation Γ_λ together with Γ_η determine the coupling between secondary and primary tensor parameters. The explicit form of these faint interactions (Aizu, 1973; Kopský, 1979*d*) can be found in the software *GI⋆KoBo*-1 and in Kopský (2001).

(4) *Changes of property tensors at a ferroic phase transition.* These changes are described by tensor parameters that depend only on the point-group-symmetry descent $G \Downarrow F$. This means that *the same principal tensor parameters and secondary tensor parameters appear in all equitranslational and in all non-equitranslational transitions with the same* $G \Downarrow F$. The only difference is that in non-equitranslational ferroic phase transitions a principal tensor parameter corresponds to a secondary ferroic order parameter. It still plays a leading role in tensor distinction of domains, since it exhibits different values in any two ferroic domain states (see Section 3.4.2.3). Changes of property tensors at ferroic phase transitions are treated in detail in the software *GI⋆KoBo*-1 and in Kopský (2001).

We note that Table 3.1.3.1 covers only those point-group symmetry descents $G \Downarrow F$ that are 'driven' by *R*-ireps of *G*. All possible point-group symmetry descents $G \Downarrow F$ are listed in Table 3.4.2.7. Principal and secondary tensor parameters of symmetry descents associated with reducible representations are combinations of tensor parameters appearing in Table 3.1.3.1 (for a detailed explanation, see the manual of the software *GI⋆KoBo*-1 and Kopský, 2000). Necessary data for treating these cases are available in the software *GI⋆KoBo*-1 and Kopský (2001).

3.1.3.3.1. *Explanation of Table 3.1.3.1*

Parent symmetry G: the short international (Hermann–Mauguin) and the Schoenflies symbol of the point group G of the parent phase are given. Subscripts specify the orientation of symmetry elements (generators) in the Cartesian crystallophysical coordinate system of the group G (see Figs. 3.4.2.3 and 3.4.2.4, and Tables 3.4.2.5 and 3.4.2.6).

R-irep Γ_η: physically irreducible representation Γ_η of the group G in the spectroscopic notation. This representation defines transformation properties of the primary order parameter η and of the principal tensor parameters. Each complex irreducible representation is combined with its complex conjugate and thus a real physically irreducible representation *R*-irep is formed. Matrices $D^{(\alpha)}$ of *R*-ireps are given explicitly in the the software *GI⋆KoBo*-1.

Table 3.1.3.2. *Symmetry descents* $G \Downarrow F_1$ *associated with two irreducible representations*

			Proper or improper		Domain states			Full or partial	
G	Γ_η	F_1	Ferroelectric	Ferroelastic	n_f	n_e	n_a	Ferroelectric	Ferroelastic
432	T_1 T_2	2_{xy}	proper improper	improper proper	12	12	12	full	full
	T_1 T_2	1	improper proper	improper proper	24	24	24	full	full
$\bar{4}3m$	T_1 T_2	m_{xy}	improper proper	improper proper	12	12	12	full	full
	T_1 T_2	1	improper proper	improper proper	24	24	24	full	full
$m\bar{3}m$	T_{1g} T_{2g}	$2_{xy}/m_{xy}$	non non	improper proper	12	0	12	non	full
	T_{1g} T_{2g}	$\bar{1}$	non non	improper proper	24	0	24	non	full
	T_{1u} T_{2u}	$m_{x\bar{y}}2_{xy}m_z$	proper improper	improper improper	12	12	6	full	partial
	T_{1u} T_{2u}	m_z	proper improper	improper improper	24	24	12	full	partial
	T_{1u} T_{2u}	1	proper improper	improper improper	48	48	24	full	partial

(La) below the symbol of the irreducible representation Γ_η indicates that the *Landau condition* is violated, hence the transition cannot be continuous (second order). The Landau condition requires the absence of the third-degree invariant polynomial of the order-parameter components (the symmetrized triple product $[\Gamma_\eta]^3$ must not contain the identity representation of G). For more details see Lyubarskii (1960), Kociński (1983, 1990), Tolédano & Tolédano (1987), Izyumov & Syromiatnikov (1990) and Tolédano & Dmitriev (1996).

(Li) below the symbol of the irreducible representation Γ_η means that the *Lifshitz condition* is violated, hence the transition to a homogeneous ferroic phase is not continuous. The Lifshitz condition demands the absence of invariant terms that couple bilinearly the order-parameter components with their spatial derivatives that are not exact differentials (the antisymmetric square $\{\Gamma_\eta\}^2$ has no representation in common with the vector representation of G). For more details see Lyubarskii (1960), Kociński (1983, 1990), Tolédano & Tolédano (1987), Izyumov & Syromiatnikov (1990) and Tolédano & Dmitriev (1996).

If there is no symbol (La) and/or (Li) below the symbol of the R-irep Γ_η (*i.e.* if both Landau and Lifshitz conditions are fulfilled), then the R-irep is called an *active representation*. In the opposite case, the R-irep is a *passive representation* (Lyubarskii, 1960; Kociński, 1983, 1990).

Standard variables: components of the order parameter in the carrier space of the irreducible representation Γ_η expressed in so-called *standard variables* (see the manual of the software *GI⋆KoBo*-1). Upper and lower indices and the typeface of standard variables allow one to identify to which irreducible representation Γ_η they belong. Standard variables of one-dimensional representations are denoted by x (Sans Serif typeface), two- or three-dimensional R-ireps by x, y or x, y, z, respectively. Upper indices $^+$ and $^-$ correspond to the lower indices g (*gerade*) and u (*ungerade*) of spectroscopic notation, respectively. The lower index specifies to which irreducible representation the variable belongs.

For multidimensional representations, a general vector of the carrier space V_η is given in the last row; this vector is invariant under the kernel of Γ_η that appears as a low-symmetry group in column F_1. The other rows contain special vectors defined by equal or zero values of some standard variables; these vectors are invariant under epikernels of Γ_η given in column F_1.

F_1: short international (Hermann–Mauguin) and Schoenflies symbol of the point group F_1 which describes the symmetry of the first single domain state of the ferroic (low-symmetry) phase. The subscripts define the orientation of symmetry elements (generators) of F_1 in the Cartesian crystallophysical coordinate system of the group G (see Figs. 3.4.2.3 and 3.4.2.4, and Tables 3.4.2.5 and 3.4.2.6). This specifies the orientation of the group F_1, which is a prerequisite for domain structure analysis (see Chapter 3.4).

n_F: number of subgroups conjugate to F_1 under G. If $n_F = 1$, the group F_1 is a normal subgroup of G (see Section 3.2.3).

Principal tensor parameters: covariant tensor components, *i.e.* linear combinations of Cartesian tensor components that transform according to the same matrix R-irep $D^{(\eta)}$ as the primary order parameter η. Principal tensor parameters are given in this form in the software *GI⋆KoBo*-1 and in Kopský (2001).

This presentation is in certain situations not practical, since property tensors are usually described by numerical values of their Cartesian components. Then it is important to know morphic Cartesian tensor components and symmetry-breaking increments of nonzero Cartesian components that appear spontaneously in the ferroic phase. The bridge between these two presentations is

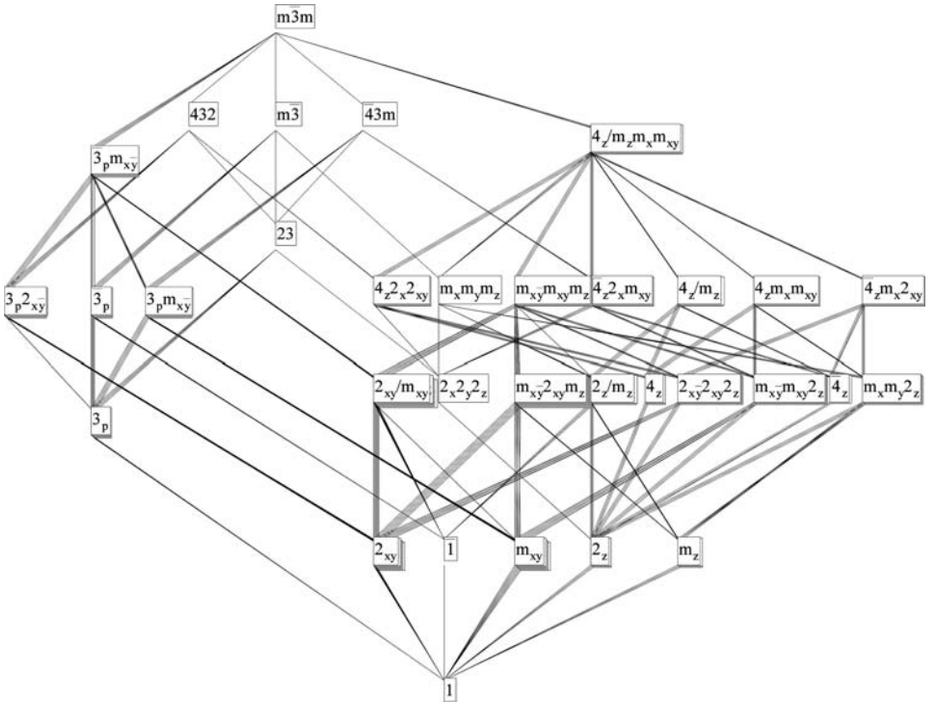

Fig. 3.1.3.1. Lattice of subgroups of the group $m\bar{3}m$. Conjugate subgroups are depicted as a pile of cards. In the software *GI⋆KoBo*-1, one can pull out individual conjugate subgroups by clicking on the pile. All conjugate subgroups are given explicitly in Table 3.4.2.7.

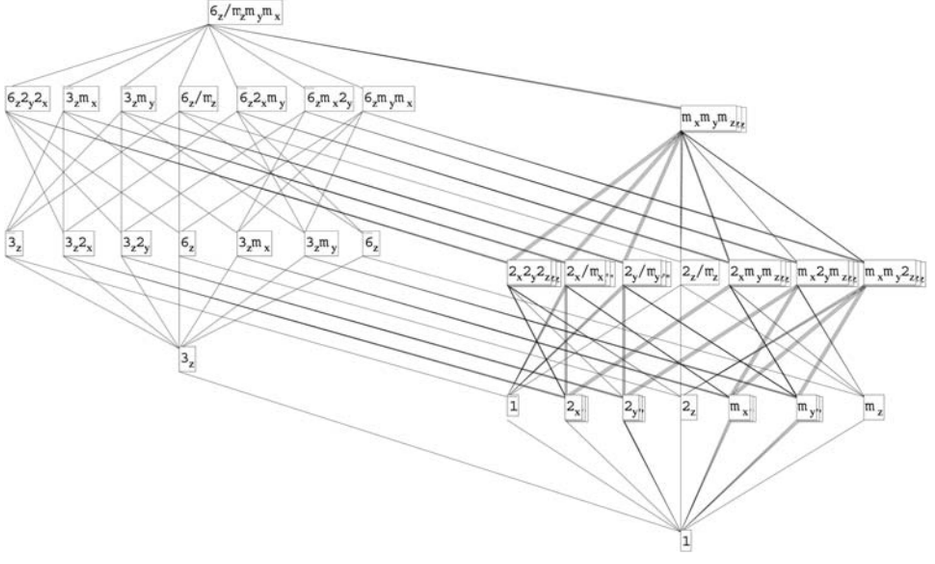

Fig. 3.1.3.2. Lattice of subgroups of the group $6/mmm$. Conjugate subgroups are depicted as a pile of cards. In the software *GI⋆KoBo*-1, one can pull out individual conjugate subgroups by clicking on the pile. All conjugate subgroups are given explicitly in Table 3.4.2.7.

provided by the *conversion equations* that express Cartesian tensor components as linear combinations of principal and secondary covariant components (for more details on tensorial covariants and conversion equations see Appendix E of the manual for *GI★KoBo*-1 and Kopský, 2001).

We illustrate the situation on a transition with symmetry descent $4_z2_x2_{xy} \Downarrow 2_x2_y2_z$. In Table 3.1.3.1, we find that the principal tensor parameter transforms according to irreducible representation B_1 with standard variable x_3. The corresponding covariant $\mathsf{u}_3 = u_1 - u_2$ can be found in Appendix E of the manual of *GI★KoBo*-1 (or in Kopský, 2001), where one also finds an invariant containing u_1 and u_2: $\mathsf{u}_{1,1} = u_1 + u_2$. The corresponding conversion equations are: $u_1 = \frac{1}{2}(\mathsf{u}_{1,1} + \mathsf{u}_3)$, $u_2 = \frac{1}{2}(\mathsf{u}_{1,1} - \mathsf{u}_3)$. In the parent phase $\mathsf{u}_3 = u_1^{(p)} - u_2^{(p)} = 0$, hence $u_1^{(p)} = u_2^{(p)} = \frac{1}{2}\mathsf{u}_{1,1}$, whereas in the ferroic phase $u_1^{(f)} = \frac{1}{2}(\mathsf{u}_{1,1} + \mathsf{u}_3) = u_1^{(p)} + \frac{1}{2}\mathsf{u}_{1,1} = u_1^{(p)} + \delta u_1$, $u_2^{(f)} = u_2^{(p)} - \frac{1}{2}\mathsf{u}_{1,1} = u_2^{(p)} + \delta u_2 = u_1^{(p)} - \delta u_1$. The symmetry-breaking increments $\delta u_1 = -\delta u_2$ describe thus the changes of the Cartesian components that correspond to the nonzero principal tensor component $u_1 - u_2$.

An analogous situation occurs frequently in trigonal and hexagonal parent groups, where $u_1 - u_2$ (or $g_1 - g_2$) transforms like the first or second component of the principal tensor parameter. In these cases, the corresponding symmetry-breaking increments of Cartesian components are again related: $\delta u_1 = -\delta u_2$ (or $\delta g_1 = -\delta g_2$).

We note that relations like $A_{11} = -A_{12} = -A_{26}$ do not imply that these components transform as the standard variable. Though these components are proportional to the principal tensor parameter in the first domain state, they cannot be transformed to corresponding components in other domain states as easily as covariant tensor components of the principal tensor parameter.

In general, it is useful to consider a tensor parameter as a vector in the carrier space of the respective representation. Then the Cartesian components are projections of this vector on the Cartesian basis of the tensor space.

The presentation of the principal tensor parameters in the column *Principal tensor parameters* of this table is a compromise: whenever conversion equations lead to simple relations between morphic Cartesian components and/or symmetry-breaking increments, we present these relations, in some cases together with corresponding covariants. In the more complicated cases, only the covariants are given. The corresponding conversion equations and labelling of covariants are given at the beginning of that part of the table which covers hexagonal and cubic parent groups G. In the main tables of the software *GI★KoBo*-1, the principal tensor parameters and the secondary tensor parameters up to rank 4 are given consistently in covariant form. Labelling of covariant components and conversion equations are given in Appendix E of the manual.

The principal tensor parameters presented in Table 3.1.3.1 represent a particular choice of property tensors for standard variables given in the second column. To save space, property tensors are selected in the following way: polarization **P** and strain u are always listed; if none of their components transform according to $D^{(\eta)}$, then components of one axial and one polar tensor (if available) appearing in Table 3.1.3.3 are given. Principal parameters of two different property tensors are separated by a semicolon. If two different components of the same property tensor transform in the same way, they are separated by a comma.

As tensor indices we use integers 1, 2, 3 instead of vector components x, y, z and contracted indices 1, 2, 3, 4, 5, 6 in matrix notation for pairs $xx, yy, zz, yz \approx zy, zx \approx xz, xy \approx yx$, respectively

Important note: To make Table 3.1.3.1 compatible with the software *GI★KoBo*-1 and with Kopský (2001), coefficients of property tensors in matrix notation with contracted indices 4, 5, 6 *do not* contain the numerical factors 2 and 4 which are usually introduced to preserve a compact form (without these factors) of linear constitutive relations [see Chapter 1.1, Nye (1985) and especially Appendices E and F of Sirotin & Shaskolskaya (1982)]. This explains the differences in matrix coefficients appearing in Table 3.1.3.1 and those presented in Chapter 1.1 or in Nye (1985) and in Sirotin & Shaskolskaya (1982). Thus *e.g.* for the symmetry descent $6_z2_x2_y \Downarrow 3_z2_x$, we find in Table 3.1.3.1 the principal tensor parameters $d_{11} = -d_{12} = -d_{26}$, whereas according to Chapter 1.1 or *e.g.* to Nye (1985) or Sirotin & Shaskolskaya (1982) these coefficients for $F_1 = 3_z2_x$ are related by equations $d_{11} = -d_{12} = -2d_{26}$.

Table 3.1.3.3. *Important property tensors*

$i = 1, 2, 3$; $\mu, \nu = 1, 2, \ldots, 6$.

Tensor components	Property	Tensor components	Property
ε	enantiomorphism		chirality
P_i	polarization	p_i	pyroelectricity
u_μ	strain	ε_{ij}	dielectric permittivity
g_μ	optical activity		
$d_{i\mu}$	piezoelectricity	$r_{i\mu}$	electro-optics
$A_{i\mu}$	electrogyration		
$\pi_{\mu\nu}$	piezo-optics	$Q_{\mu\nu}$	electrostriction

Property tensors and symbols of their components that can be found in Table 3.1.3.1 are given in the left-hand half of Table 3.1.3.3. The right-hand half presents other tensors that transform in the same way as those on the left and form, therefore, covariant tensor components of the same form as those given in the column *Principal tensor parameters*. Principal and secondary tensor parameters for all property tensors that appear in Table 3.1.3.3 are available in the software *GI★KoBo*-1.

n_f: number of ferroic single domain states that differ in the primary order parameter η and in the principal tensor parameters.

n_a: number of ferroelastic single domain states. If $n_a = n_f$, $n_a < n_f$ or $n_a = 1$, the ferroic phase is, respectively, a full, partial or non-ferroelastic one.

n_e: number of ferroelectric single domain states. If $n_e = n_f$, $n_e < n_f$ or $n_e = 0, 1$, the ferroic phase is, repectively, a full, partial or non-ferroelectric one ($n = 0$ or $n = 1$ correspond to a non-polar or to a polar parent phase, respectively) (see Section 3.4.2).

3.1.3.4. *Examples*

Example 3.1.3.4.1. Phase transition in triglycine sulfate (TGS). Assume that the space groups of both parent (high-symmetry) and ferroic (low-symmetry) phases are known: $\mathcal{G} = P2_1/c$ (C_{2h}^5), $\mathcal{F}_1 = P2_1$ (C_2^2). The same number of formula units in the primitive unit cell in both phases suggests that the transition is an equitranslational one. This conclusion can be checked in the lattice of equitranslational subgroups of the software *GI★KoBo*-1. There we find for the low-symmetry space group the symbol $P112_1(\mathbf{b}/4)$, where the vector in parentheses expresses the shift of the origin with respect to the conventional origin given in *IT* A (2002).

In Table 3.1.3.1, one finds that the corresponding point-group-symmetry descent $2_z/m_z \Downarrow 2_z$ is associated with irreducible representation $\Gamma_\eta = A_u$. The corresponding principal tensor parameters of lowest rank are the pseudoscalar ε (enantiomorphism or chirality) and the vector of spontaneous polarization with one nonzero morphic component P_3 – the transition is a proper ferroelectric one. The non-ferroelastic ($n_a = 1$) full ferroelectric phase has two ferroelectric domain states ($n_f = n_e = 2$). Other principal tensor parameters (morphic tensor components that transform according to Γ_η) are available in the software *GI★KoBo*-1: g_1, g_2, g_3, g_6; $d_{31}, d_{32}, d_{33}, d_{36}, d_{14}, d_{15}, d_{24}, d_{25}$. Property tensors with these components are listed in Table 3.1.3.3. As shown in Section 3.4.2, all these components

change sign when one passes from one domain state to the other. Since there is no intermediate group between G and F, there are no secondary tensor parameters.

Example 3.1.3.4.2. Phase transitions in barium titanate ($BaTiO_3$). We shall illustrate the solution of the inverse Landau problem and the need to correlate the crystallographic system with the Cartesian crystallophysical coordinate system. The space-group type of the parent phase is $\mathcal{G} = Pm\bar{3}m$, and those of the three ferroic phases are $\mathcal{F}_1^{(1)} = P4mm$, $\mathcal{F}_1^{(2)} = Cm2m$, $\mathcal{F}_1^{(3)} = R3m$, all with one formula unit in the primitive unit cell.

This information is not complete. To perform mode analysis, we must specify these space groups by saying that the lattice symbol P in the first case and the lattice symbol R in the third case are given with reference to the cubic crystallographic basis (**a**, **b**, **c**), while lattice symbol C in the second case is given with reference to crystallographic basis [(**a** − **b**), (**a** + **b**), **c**]. If we now identify vectors of the cubic crystallographic basis with vectors of the Cartesian basis by $\mathbf{a} = a\mathbf{e}_x$, $\mathbf{b} = a\mathbf{e}_y$, $\mathbf{c} = a\mathbf{e}_z$, where $\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ are three orthonormal vectors, we can see that the corresponding point groups are $F_1^{(1)} = 4_z m_x m_{xy}$, $F_1^{(2)} = m_{x\bar{y}} 2_{xy} m_z$, $F_1^{(3)} = 3_p m_{x\bar{y}}$.

Notice that without specification of crystallographic bases one could interpret the point group of the space group $Cm2m$ as $m_x 2_y m_z$. Bases are therefore always specified in lattices of equitranslational subgroups of the space groups that are available in the software *GI★KoBo*-1, where we can check that all three symmetry descents are equitranslational.

In Table 3.1.3.1, we find that these three ferroic subgroups are epikernels of the R-irep $\Gamma_\eta = T_{1u}$ with the following principal tensor components: P_3, $P_1 = P_2$, $P_1 = P_2 = P_3$, respectively. Other principal tensor parameters can be found in the main tables of the software *GI★KoBo*-1. The knowledge of the representation Γ_η allows one to perform soft-mode analysis (see *e.g.* Rousseau *et al.*, 1981).

For the tetragonal ferroelectric phase with $F_1 = 4_z m_x m_y$, we find in Fig. 3.1.3.1 an intermediate group $L_1 = 4_z/m_z m_x m_{xy}$. In Table 3.1.3.1, we check that this is an epikernel of the R-irep E_g with secondary tensor parameter δu_3. This phase is a full (proper) ferroelectric and partial ferroelastic one.

More details about symmetry aspects of structural phase transitions can be found in monographs by Izyumov & Syromiatnikov (1990), Kociński (1983, 1990), Landau & Lifshitz (1969), Lyubarskii (1960), Tolédano & Dmitriev (1996) and Tolédano & Tolédano (1987). Group–subgroup relations of space groups are treated extensively in *IT* A1 (2003).

3.1.4. Example of a table for non-equitranslational phase transitions

By J.-C. Tolédano

In the preceding Section 3.1.3, a systematic tabulation of possible symmetry changes was provided for the class of equitranslational phase transitions. This tabulation derives from the principles described in Section 3.1.2, and relates the enumeration of the symmetry changes at structural transitions to the characteristics of the irreducible representations of the space group $\mathcal{G}$ of the 'parent' (highest-symmetry) phase adjacent to the transition. Systematic extension of this type of tabulation to the general case of transitions involving both a decrease of translational and of point-group symmetry has been achieved by several groups (Tolédano & Tolédano, 1976, 1977, 1980, 1982; Stokes & Hatch, 1988). The reader can refer, in particular, to the latter reference for an exhaustive enumeration of the characteristics of possible transitions. An illustration of the results obtained for a restricted class of parent phases (those associated with the point symmetry $4/m$ and to a simple Bravais lattice P) is presented here.

In order to clarify the content Table 3.1.4.1, let us recall (*cf.* Section 3.1.2) that Landau's theory of continuous phase transitions shows that the order parameter of a transition transforms according to a physically irreducible representation of the space group $\mathcal{G}$ of the high-symmetry phase of the crystal. A physically irreducible representation is either a real irreducible representation of $\mathcal{G}$ or the direct sum of two complex-conjugate irreducible representations of $\mathcal{G}$. To classify the order-parameter symmetries of all possible transitions taking place between a given parent (high-symmetry) phase and another (low-symmetry) phase, it is therefore necessary, for each parent space group, to list the various relevant irreducible representations.

Each irreducible representation of a given space group can be denoted $\Gamma_n(k^*)$ and identified by two quantifies. The star k^*, represented by a vector linking the origin of reciprocal space to a point of the first Brillouin zone, specifies the translational symmetry properties of the basis functions of $\Gamma_n(k^*)$. The dimension of $\Gamma_n(k^*)$ is equal to the number of components of the order parameter of the phase transition considered. A given space group has an infinite number of irreducible representations. However, physical considerations restrict a systematic enumeration to only a few irreducible representations. The restrictions arise from the fact that one focuses on continuous (or almost continuous) transitions between strictly periodic crystal structures (*i.e.* in particular, incommensurate phases are not considered), and have been thoroughly described previously (Tolédano & Tolédano, 1987, and references therein).

3.1.5. Microscopic aspects of structural phase transitions and soft modes

By J. F. Scott

3.1.5.1. *Introduction*

Phase transitions in crystals are most sensitively detected *via* dynamic techniques. Two good examples are ultrasonic attenuation and internal friction. Unfortunately, while often exquisitely sensitive to subtle second-order phase transitions [*e.g.* the work of Spencer *et al.* (1970) on $BaMnF_4$], they provide no real structural information on the lattice distortions that occur at such phase transitions, or even convincing evidence that a real phase transition has occurred (*e.g.* transition from one long-range thermodynamically stable ordered state to another). It is not unusual for ultrasonic attenuation to reveal a dozen reproducible anomalies over a small temperature range, none of which might be a phase transition in the usual sense of the phrase. At the other extreme are detailed structural analyses *via* X-ray or neutron scattering, which give unambiguous lattice details but often totally miss small, nearly continuous rigid rotations of light ions, such as hydrogen bonds or oxygen or fluorine octahedra or tetrahedra. Intermediate between these techniques are phonon spectroscopies, notably infrared (absorption or reflection) and Raman techniques. The latter has developed remarkably over the past thirty years since the introduction of lasers and is now a standard analytical tool for helping to elucidate crystal structures and phase transitions investigated by chemists, solid-state physicists and materials scientists.

3.1.5.2. *Displacive phase transitions*

3.1.5.2.1. *Landau–Devonshire theory*

Landau (1937) developed a simple mean-field theory of phase transitions which implicitly assumes that each atom or ion in a system exerts a force on the other particles that is independent of the distance between them (see Section 3.1.2.2). Although this is a somewhat unphysical crude approximation to the actual forces, which are strongly dependent upon interparticle spacings, it allows the forces of all the other particles in the system to be replaced mathematically by an effective 'field', and for the