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

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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 $\mathrm{Ker}\ \Gamma_\eta$, 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 $\mathrm{Ker}\ \Gamma_\eta$. 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: $4_z2_x2_{xy}$ D_{4z}								
A_2	x_2	4_z	C_{4z}	1	P_3	2	1	2
B_1	x_3	$2_x2_y2_z$	D_2	1	$\delta u_1 = -\delta u_2$	2	2	0
B_2	x_4	$2_{x\bar{y}}2_{xy}2_z$	$\hat{D}_{2z}$	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: $4_zm_xm_{xy}$ 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	$m_xm_y2_z$	C_{2vz}	1	$\delta u_1 = -\delta u_2$	2	2	1
B_2	x_4	$m_{x\bar{y}}m_{xy}2_z$	$\hat{C}_{2vz}$	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: $\bar{4}_z2_xm_{xy}$ 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	$2_x2_y2_z$	D_2	1	ε; $\delta u_1 = -\delta u_2$	2	2	0
B_2	x_4	$m_{x\bar{y}}m_{xy}2_z$	$\hat{C}_{2vz}$	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: $\bar{4}_zm_x2_{xy}$ $\hat{D}_{2dz}$								
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	$m_xm_y2_z$	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: $4_z/m_zm_xm_{xy}$ 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^+	$m_xm_ym_z$	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^-	$4_z2_x2_{xy}$	D_{4z}	1	ε; $g_1 = g_2$, g_3; $d_{14} = -d_{25}$	2	1	0
A_{2u}	x_2^-	$4_zm_xm_{xy}$	C_{4vz}	1	P_3	2	1	2
B_{1u}	x_3^-	$\bar{4}_z2_xm_{xy}$	D_{2dz}	1	$g_1 = -g_2$; $d_{14} = d_{25}$, d_{36}	2	1	0
B_{2u}	x_4^-	$\bar{4}_zm_x2_{xy}$	$\hat{D}_{2dz}$	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	$(x_1^-, 0)$	$2_xm_ym_z$	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: 3_z C_3								
E	(x_1, y_1)	1	C_1	1	(P_1, P_2)	3	3	3
					$(u_1 - u_2, -2u_6)$, $(u_4, -u_5)$			
(La, Li)					$\delta u_1 = -\delta u_2$			
Parent symmetry G: $\bar{3}_z$ C_{3i}								
A_u	x_1^-	3_z	C_3	1	ε; P_3	2	1	2
E_g	(x_1^+, y_1^+)	$\bar{1}$	C_i	1	$(u_1 - u_2, -2u_6)$, $(u_4, -u_5)$	3	3	0
(La)					$\delta u_1 = -\delta u_2$			
E_u	(x_1^-, y_1^-)	1	C_1	1	(P_1, P_2)	6	3	6
Parent symmetry G: 3_z2_x 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: 3_zm_x 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 (La, Li)	(x_2, y_2)	2_z	C_{2z}	1	$(u_1-u_2, 2u_6)$ $\delta u_1=-\delta u_2$	3	3	1
E_1 (Li)	(x_1, y_1)	1	C_1	1	(P_1, P_2) $(u_4, -u_5)$	6	6	6
Parent symmetry G: $\bar{6}_z$ C_{3h}								
A''	x_3	3_z	C_3	1	ε; P_3	2	1	2
E' (La)	(x_2, y_2)	m_z	C_{sz}	1	(P_2, P_1) $(u_1-u_2, 2u_6)$ $\delta u_1=-\delta u_2$	3	3	3
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} (La)	(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
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	$(g_1-g_2, 2g_6)$ $g_1=-g_2, g_6$ $(2d_{36}, d_{32}-d_{31})$ $d_{32}=-d_{31}, d_{36}$ $(d_{14}+d_{25}, d_{24}-d_{15})$ $d_{14}=d_{25}, d_{24}=-d_{15}$	6	3	2
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: $6_z2_x2_y$ D_6								
A_2	x_2	6_z	C_6	1	P_3	2	1	2
B_1	x_3	3_z2_x	D_{3x}	1	$d_{11} = -d_{12} = -d_{26}$	2	1	0
B_2	x_4	3_z2_y	D_{3y}	1	$d_{22} = -d_{21} = -d_{16}$	2	1	0
E_2	$(x_2, 0)$	$2_x2_y2_z$	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: $6_zm_xm_y$ 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_zm_x	C_{3vx}	1	$d_{22} = -d_{21} = -d_{16}$	2	1	1
B_1	x_4	3_zm_y	C_{3vy}	1	$d_{11} = -d_{12} = -d_{26}$	2	1	1
E_2	$(x_2, 0)$	$m_xm_y2_z$	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: $\bar{6}_z2_xm_y$ 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_z2_x	D_{3x}	1	ε; $g_1 = g_2$, g_3; $d_{14} = -d_{25}$	2	1	0
A_2''	x_4	3_zm_y	C_{3vy}	1	P_3	2	1	2
E'	$(x_2, 0)$	$2_xm_ym_z$	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: $\bar{6}_zm_x2_y$ $\hat{D}_{3h}$								
A_2'	x_2	$\bar{6}_z$	C_{3h}	1	$d_{11} = -d_{12} = -d_{26}$	2	1	0
A_2''	x_3	3_zm_x	C_{3vx}	1	P_3	2	1	2
A_1'	x_4	3_z2_y	D_{3y}	1	ε; $g_1 = g_2$, g_3; $d_{14} = -d_{25}$	2	1	0
E'	$(x_2, 0)$	$m_x2_ym_z$	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: $6_z/m_zm_xm_y$ 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^+	$\bar{3}_zm_x$	D_{3dx}	1	$A_{11} = -A_{12} = -A_{26}$	2	1	0
B_{2g}	x_4^+	$\bar{3}_zm_y$	D_{3dy}	1	$A_{22} = -A_{21} = -A_{16}$	2	1	0
A_{1u}	x_1^-	$6_z2_x2_y$	D_6	1	ε; $g_1 = g_2$, g_3; $d_{14} = -d_{25}$	2	1	0
A_{2u}	x_2^-	$6_zm_xm_y$	C_{6v}	1	P_3	2	1	2
B_{1u}	x_3^-	$\bar{6}_z2_xm_y$	D_{3h}	1	$d_{11} = -d_{12} = -d_{26}$	2	1	0
B_{2u}	x_4^-	$\bar{6}_zm_x2_y$	$\hat{D}_{3h}$	1	$d_{22} = -d_{21} = -d_{16}$	2	1	0
E_{2g}	$(x_2^+, 0)$	$m_xm_ym_z$	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}	$(x_1^-, 0)$	$2_xm_ym_z$	C_{2vx}	3	P_1	6	3	6
	$(0, y_1^-)$	$m_x2_ym_z$	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}	$(x_2^-, 0)$	$2_x2_y2_z$	D_2	3	$\delta g_1 = -\delta g_2$; d_{36}, $\delta d_{14} = \delta d_{25}$	6	3	0
	$(0, y_2^-)$	$m_xm_y2_z$	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 nonpolar 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