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*$\star$*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*$\star$*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*$\star$*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*$\star$*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*$\star$*KoBo*-1 and Kopský, 2000). Necessary data for treating these cases are available in the software *GI*$\star$*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*$\star$*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

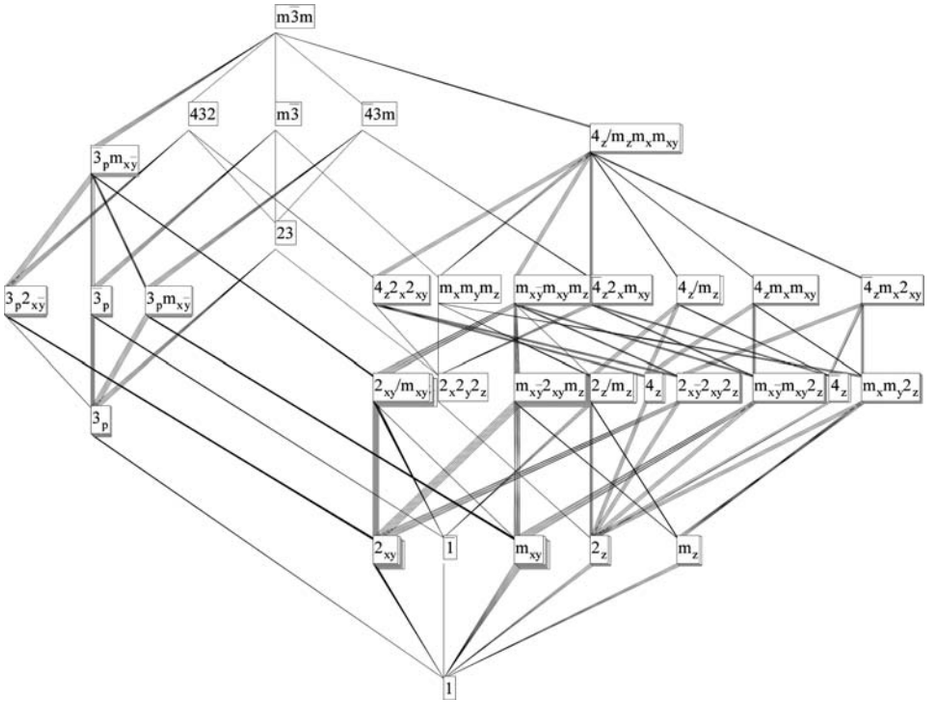

Fig. 3.1.3.1. Lattice of subgroups of the group $m\bar{3}m$. Conjugate subgroups are depicted as a pile of cards. In the software *GI⋆KoBo*-1, one can pull out individual conjugate subgroups by clicking on the pile.

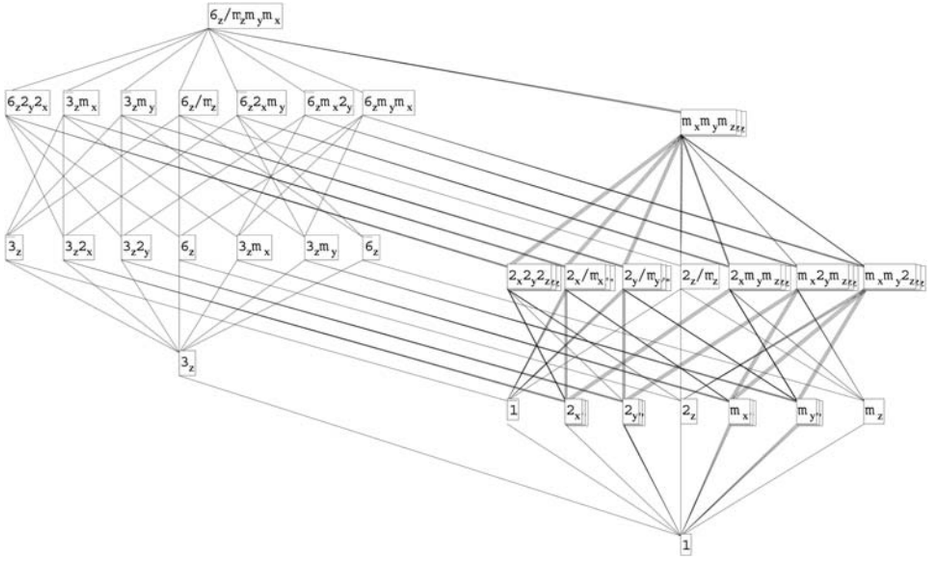

Fig. 3.1.3.2. Lattice of subgroups of the group $6/mmm$. Conjugate subgroups are depicted as a pile of cards. In the software *GI⋆KoBo*-1, one can pull out individual conjugate subgroups by clicking on the pile.

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 (2005).

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