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domain states have the same symmetry (stabilizer in G). The number n_F of subgroups conjugate to F_1 in G is $n_F = [G : N_G(F_1)] = |G| : |N_G(F_1)|$ [see equation (3.4.2.36)] and the number d_F of principal domain states with the same symmetry is $d_F = [N_G(F_1) : F_1] = |N_G(F_1)| : |F_1|$ [see equation (3.4.2.35)]. There are three possible cases:

(i) $N_G(F_1) = G$. There are no subgroups conjugate to F_1 and the symmetry group F_i (stabilizer of $\mathbf{S}_i$ in G) of all principal domain states $\mathbf{S}_1, \mathbf{S}_2, \ldots, \mathbf{S}_n$ is equal to F_i for all $i = 1, 2, \ldots, n$; hence domain states cannot be distinguished by their symmetry. The group F_1 is a normal subgroup of G, $F_1 \triangleleft G$ (see Section 3.2.3.2). This is always the case if there are just two single-domain states $\mathbf{S}_1$, $\mathbf{S}_2$, *i.e.* if the index of F_1 in G equals two, $[G : F_1] = |G| : |F_1| = 2$.

(ii) $N_G(F_1) = F_1$. Then any two domain states $\mathbf{S}_i$, $\mathbf{S}_k$ have different symmetry groups (stabilizers), $\mathbf{S}_i \neq \mathbf{S}_k \Leftrightarrow F_i \neq F_k$, *i.e.* there is a one-to-one correspondence between single-domain states and their symmetries, $\mathbf{S}_i \Leftrightarrow F_i$. In this case, principal domain states $\mathbf{S}_i$ can be specified by their symmetries F_i, $i = 1, 2, \ldots, n$. The number n_F of different groups conjugate to F_1 is equal to the index $[G : F_1] = |G| : |F_1| = n$.

(iii) $F_1 \subset N_G(F_1) \subset G$. Some, but not all, domain states $\mathbf{S}_i$, $\mathbf{S}_k$ have identical symmetry groups (stabilizers) $F_i = F_k$. The number d_F of domain states with the same symmetry group is $d_F = [N_G(F_1) : F_1] = |N_G(F_1)| : |F_1|$ [see equation (3.4.2.35)], $1 < d_F < n$. The number n_F of different groups conjugate to F_1 is equal to the index $n_F = [G : N_G(F_1)] = |G| : |N_G(F_1)|$ [see equation (3.4.2.36)] and in this case $1 < n_F < n$. It always holds that $n_F d_F = n$ [see equation (3.4.2.37)].

$K_G(F_1, g_{1j})$: *twinning group of a domain pair* ($\mathbf{S}_1$, $\mathbf{S}_j$). This group is defined in Section 3.4.3.2. It can be considered a colour (polychromatic) group involving c colours, where $c = [K_{1j} : F_1]$, and is, therefore, defined by *two* groups K_{1j} *and* F_1, and its full symbol is $K_{1j}(F_1)$. In this column only K_{1j} is given, since F_1 appears in the second column of the table.

If the group symbol of K_{1j} contains generators with the star symbol, *, which signifies transposing operations of the domain pair ($\mathbf{S}_1$, $\mathbf{S}_j$), then the symbol $K_{1j}(F_1)$ denotes a dichromatic ('black-and-white') group signifying a completely transposable domain pair. In this special case, just the symbol K_{1j} containing stars * specifies the group F_1 unequivocally.

The number in parentheses after the group symbol of K_{1j} is equal to the number of twinning groups K_{1k} equivalent with K_{1j}.

In the continuum description, a twinning group is significant in at least in two instances:

(1) A twinning group $K_{1j}(F_1)$ specifies the distinction of two domain states $\mathbf{S}_1$ and $\mathbf{S}_j = g_{1j}\mathbf{S}_1$, where $g_{1j} \in G$ (see Sections 3.4.3.2 and 3.4.3.4).

(2) A twinning group $K_{1j}(F_1)$ may assist in signifying classes of equivalent domain pairs (orbits of domain pairs). In most cases, to a twinning group F_{1j} there corresponds just one class of equivalent domain pairs (an orbit) $G(\mathbf{S}_1, \mathbf{S}_j)$; then a twinning group can represent this class of equivalent domain pairs. Nevertheless, in some cases two or more classes of equivalent domain pairs have a common twinning group. Then one has to add a switching operation g_{1j} to the twinning group, $K_{1j}(F_1, g_{1j})$ (see the end of Section 3.4.3.2). In this way, classes of equivalent domain pairs $G(\mathbf{S}_1, \mathbf{S}_j)$ are denoted in synoptic Tables 3.4.2.7 and 3.4.3.6.

Twinning groups given in column K_{1j} thus specify *all G-orbits of domain pairs*. The number of G-orbits and representative domain pairs for each orbit are determined by double cosets of group F_1 (see Section 3.4.3.2). Representative domain pairs from each orbit of domain pairs are further analysed in synoptic Table 3.4.3.4 (non-ferroelastic domain pairs) and in synoptic Table 3.4.3.6 (ferroelastic domain pairs).

The set of the twinning groups K_{1j} given in this column is analogous to the concept of a *complete twin* defined as 'an edifice comprising in addition to an original crystal (domain state $\mathbf{S}_1$) as many twinned crystals (domain states $\mathbf{S}_j$) as there are possible twin laws' (see Curien & Le Corre, 1958). If a traditional definition of a twin law ['a geometrical relationship between two crystal components of a twin', see Section 3.3.2 and Koch (2004); Curien & Le Corre (1958)] is applied *sensu stricto* to domain twins then one gets the following correspondence:

(i) a twin law of a non-ferroelastic domain twin is specified by the twinning group K_{1j} (see Section 3.4.3.3 and Table 3.4.3.4);

(ii) two twin laws of two compatible ferroelastic domain twins, resulting from one ferroelastic single-domain pair $\{\mathbf{S}_1, \mathbf{S}_j\}$, are specified by two layer groups $\bar{\mathsf{J}}_{1j}$ associated with the twinning group K_{1j} of this ferroelastic single-domain pair $\{(\mathbf{S}_1, \mathbf{S}_j)\}$ (see Section 3.4.3.4 and Table 3.4.3.6).

n: *number of principal single-domain states*, the finest subdivision of domain states in a continuum description, $n = [G : F_1] = |G| : |F_1|$ [see equation (3.4.2.11)].

d_F: *number of principal domain states with the same symmetry group (stabilizer)*, $d_F = [N_G(F_1) : F_1] = |N_G(F_1)| : |F_1|$ [see equation (3.4.2.35)]. If $d_F > 1$, then the group F_1 does not specify the first single-domain state $\mathbf{S}_1$. The number n_F of subgroups conjugate with F_1 is $n_F = n : d_F$.

n_e: *number of ferroelectric single-domain states*, $n_e = [G : C_1] = |G| : |C_1|$, where C_1 is the stabilizer (in G) of the spontaneous polarization in the first domain state $\mathbf{S}_1$ [see equation (3.4.2.32)]. The number d_e of principal domain states compatible with one ferroelectric domain state (degeneracy of ferroelectric domain states) equals $d_e = [C_1 : F_1] = |C_1| : |F_1|$ [see equation (3.4.2.33)].

Aizu's classification of ferroelectric phases (Aizu, 1969; see Table 3.4.2.3): $n_e = n$, fully ferroelectric; $1 < n_e < n$, partially ferroelectric; $n_e = 1$, non-ferroelectric, the parent phase is polar and the spontaneous polarization in the ferroic phase is the same as in the parent phase; $n_e = 0$, non-ferroelectric, parent phase is non-polar.

n_a: *number of ferroelastic single-domain states*, $n_a = [G : A_1] = |G| : |A_1|$, where A_1 is the stabilizer (in G) of the spontaneous strain in the first domain state $\mathbf{S}_1$ [see equation (3.4.2.28)]. The number d_a of principal domain states compatible with one ferroelastic domain state (degeneracy of ferroelastic domain states) is given by $d_a = [A_1 : F_1] = |A_1| : |F_1|$ [see equation (3.4.2.29)].

Aizu's classification of ferroelastic phases (Aizu, 1969; see Table 3.4.2.3): $n_a = n$, fully ferroelastic; $1 < n_a < n$, partially ferroelastic; $n_e = 1$, non-ferroelastic.

Example 3.4.2.5. Orthorhombic phase of perovskite crystals. The parent phase has symmetry $G = m\bar{3}m$ and the symmetry of the ferroic orthorhombic phase is $F_1 = m_{x\bar{y}}2_{xy}m_z$. In Table 3.4.2.7, we find that $n = n_e$, *i.e.* the phase is fully ferroelectric. Then we can associate with each principal domain state a spontaneous polarization. In column K_{1j} there are four twinning groups. As explained in Section 3.4.3, these groups represent four 'twin laws' that can be characterized by the angle between the spontaneous polarization in single-domain state $\mathbf{S}_1$ and $\mathbf{S}_j$, $j = 2, 3, 4, 5$. If we choose $\mathbf{P}^{(1)}_{(s)}$ along the direction [110] (F_1 does not specify unambiguously this direction, since $d_F = 2$!), then the angles between $\mathbf{P}^{(1)}_{(s)}$ and $\mathbf{P}^{(j)}_{(s)}$, representing the 'twin law' for these four twinning groups $m\bar{3}m(m_{zx})$, $m\bar{3}m(2_{zx})$, $4_z/m_z m_x m_{xy}$, $m_{x\bar{y}}m^\star_{xy}m_z$, are, respectively, 60, 120, 90 and 180°.

3.4.2.5. *Basic (microscopic) domain states and their partition into translation subsets*

The examination of principal domain states performed in the continuum approach can be easily generalized to a *microscopic description*. Let us denote the *space-group* symmetry of the parent (high-symmetry) phase by $\mathcal{G}$ and the space group of the

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Table 3.4.2.7. *Group–subgroup symmetry descents* $G \supset F_1$

G: point-group symmetry of parent phase; F_1: point-group symmetry of single-domain state $\mathbf{S}_1$; Γ_η: representation of G; $N_G(F_1)$: normalizer of F_1 in G; $K_G(F_1, g_{1j})$: twinning groups, $g_{1j} \in G$; n: number of principal single-domain states; d_F: number of principal domain states with the same symmetry; n_e: number of ferroelectric single-domain states; n_a: number of ferroelastic single-domain states.

G	F_1	Γ_η	$N_G(F_1)$	$K_G(F_1, g_{1j})$	n	d_F	n_e	n_a
$\bar{\mathbf{1}}$	1	A_u	$\bar{1}$	$\bar{1}^\star$	2	2	2	1
$\mathbf{2}_{\boldsymbol{u}}$†	1	B	2_u	$2_u^\star$	2	2	2	2
$\boldsymbol{m_u}$†	1	A''	m_u	$m_u^\star$	2	2	2	2
$\mathbf{2}_{\boldsymbol{u}}/\boldsymbol{m_u}$†	m_u	B_u	$2_u/m_u$	$2_u^\star/m_u$	2	2	2	1
	2_u	A_u	$2_u/m_u$	$2_u/m_u^\star$	2	2	2	1
	$\bar{1}$	B_g	$2_u/m_u$	$2_u^\star/m_u^\star$	2	2	0	2
	1	Reducible	$2_u/m_u$	$m_u^\star$, $2_u^\star$, $\bar{1}^\star$	4	4	4	2
$\mathbf{2}_x\mathbf{2}_y\mathbf{2}_z$	2_z	B_{1g}	$2_x2_y2_z$	$2_x^\star 2_y^\star 2_z$	2	2	2	2
	2_x	B_{3g}	$2_x2_y2_z$	$2_x 2_y^\star 2_z^\star$	2	2	2	2
	2_y	B_{2g}	$2_x2_y2_z$	$2_x^\star 2_y 2_z^\star$	2	2	2	2
	1	Reducible	$2_x2_y2_z$	$2_z^\star$, $2_x^\star$, $2_y^\star$	4	4	4	4
$\boldsymbol{m_x m_y}\mathbf{2}_z$	m_x	B_2	$m_xm_y2_z$	$m_x m_y^\star 2_z^\star$	2	2	2	2
	m_y	B_1	$m_xm_y2_z$	$m_x^\star m_y 2_z^\star$	2	2	2	2
	2_z	A_2	$m_xm_y2_z$	$m_x^\star m_y^\star 2_z$	2	2	1	2
	1	Reducible	$m_xm_y2_z$	$m_x^\star$, $m_y^\star$, $2_z^\star$	4	2	4	4
$\boldsymbol{m_x m_y m_z}$	$m_xm_y2_z$	B_{1u}	$m_xm_ym_z$	$m_x m_y m_z^\star$	2	2	2	1
	$2_xm_ym_z$	B_{3u}	$m_xm_ym_z$	$m_x^\star m_y m_z$	2	2	2	1
	$m_x2_ym_z$	B_{2u}	$m_xm_ym_z$	$m_x m_y^\star m_z$	2	2	2	1
	$2_x2_y2_z$	A_{1u}	$m_xm_ym_z$	$m_x^\star m_y^\star m_z^\star$	2	2	0	1
	$2_z/m_z$	B_{1g}	$m_xm_ym_z$	$m_x^\star m_y^\star m_z$	2	2	0	2
	$2_x/m_x$	B_{3g}	$m_xm_ym_z$	$m_x m_y^\star m_z^\star$	2	2	0	2
	$2_y/m_y$	B_{2g}	$m_xm_ym_z$	$m_x^\star m_y m_z^\star$	2	2	0	2
	m_z	Reducible	$m_xm_ym_z$	$2_x^\star m_y^\star m_z$, $m_x^\star 2_y^\star m_z$, $2_z^\star/m_z$	4	4	4	2
	m_x	Reducible	$m_xm_ym_z$	$m_x m_y^\star 2_z^\star$, $m_x 2_y^\star m_z^\star$, $2_x^\star/m_x$	4	4	4	2
	m_y	Reducible	$m_xm_ym_z$	$m_x^\star m_y 2_z^\star$, $2_x^\star m_y m_z^\star$, $2_y^\star/m_y$	4	4	4	2
	2_z	Reducible	$m_xm_ym_z$	$m_x^\star m_y^\star 2_z$, $2_x^\star 2_y^\star 2_z$, $2_z/m_z^\star$	4	4	2	2
	2_x	Reducible	$m_xm_ym_z$	$2_x m_y^\star m_z^\star$, $2_x 2_y^\star 2_z^\star$, $2_x/m_x^\star$	4	4	2	2
	2_y	Reducible	$m_xm_ym_z$	$m_x^\star 2_y m_z^\star$, $2_x^\star 2_y 2_z^\star$, $2_y/m_y^\star$	4	4	2	2
	$\bar{1}$	Reducible	$m_xm_ym_z$	$2_z^\star/m_z^\star$, $2_x^\star/m_x^\star$, $2_y^\star/m_y^\star$	4	4	0	4
	1	Reducible	$m_xm_ym_z$	$m_z^\star$, $m_x^\star$, $m_y^\star$, $2_z^\star$, $2_x^\star$, $2_y^\star$, $\bar{1}^\star$	8	8	8	4
$\mathbf{4}_z$	2_z	B	4_z	$4_z^\star$	2	2	1	2
	1	${}^1E \oplus {}^2E$	4_z	4_z, $2_z^\star$	4	4	4	4
$\bar{\mathbf{4}}_z$	2_z	B	$\bar{4}_z$	$\bar{4}_z^\star$	2	2	2	2
	1	${}^1E \oplus {}^2E$	$\bar{4}_z$	$\bar{4}_z$, $2_z^\star$	4	2	4	4
$\mathbf{4}_z/\boldsymbol{m_z}$	$\bar{4}_z$	B_u	$4_z/m_z$	$4_z^\star/m_z^\star$	2	2	0	1
	4_z	A_u	$4_z/m_z$	$4_z/m_z^\star$	2	2	2	1
	$2_z/m_z$	B_g	$4_z/m_z$	$4_z^\star/m_z$	2	2	0	2
	m_z	${}^1E_u \oplus {}^2E_u$	$4_z/m_z$	$4_z/m_z$, $2_z^\star/m_z$	4	4	4	2
	2_z	Reducible	$4_z/m_z$	$\bar{4}_z^\star$, $4_z^\star$, $2_z/m_z^\star$	4	4	2	2
	$\bar{1}$	${}^1E_g \oplus {}^2E_g$	$4_z/m_z$	$4_z/m_z$, $2_z^\star/m_z^\star$	4	4	0	4
	1	Reducible	$4_z/m_z$	$\bar{4}_z$, 4_z, $m_z^\star$, $2_z^\star$, $\bar{1}^\star$	8	8	8	4
$\mathbf{4}_z\mathbf{2}_x\mathbf{2}_{xy}$	4_z	A_2	$4_z2_x2_{xy}$	$4_z 2_x^\star 2_{xy}^\star$	2	2	2	1
	$2_{x\bar{y}}2_{xy}2_z$	B_2	$4_z2_x2_{xy}$	$4_z^\star 2_x^\star 2_{xy}$	2	2	0	2
	$2_x2_y2_z$	B_1	$4_z2_x2_{xy}$	$4_z^\star 2_x 2_{xy}^\star$	2	2	0	2
	2_{xy} $(2_{x\bar{y}})$	E	$2_{x\bar{y}}2_{xy}2_z$	$4_z2_x2_{xy}$, $2_{x\bar{y}}^\star 2_{xy} 2_z^\star$	4	2	2	2
	2_z	Reducible	$4_z2_x2_{xy}$	$4_z^\star$, $2_x^\star 2_y^\star 2_z$, $2_{x\bar{y}}^\star 2_{xy}^\star 2_z$	4	4	2	2
	2_x (2_y)	E	$2_{x\bar{y}}2_{xy}2_z$	$4_z2_x2_{xy}$, $2_x 2_y^\star 2_z^\star$	4	2	2	2
	1	E	$4_z2_x2_{xy}$	4_z, $2_z^\star$, $2_x^\star(2)$, $2_{xy}^\star(2)$	8	8	8	8
$\mathbf{4}_z\boldsymbol{m_x m_{xy}}$	4_z	A_2	$4_zm_xm_{xy}$	$4_z m_x^\star m_{xy}^\star$	2	2	1	1
	$m_{x\bar{y}}m_{xy}2_z$	B_2	$4_zm_xm_{xy}$	$4_z^\star m_x^\star m_{xy}$	2	2	1	2
	$m_xm_y2_z$	B_1	$4_zm_xm_{xy}$	$4_z^\star m_x m_{xy}^\star$	2	2	1	2
	m_{xy} $(m_{x\bar{y}})$	E	$m_{x\bar{y}}m_{xy}2_z$	$4_zm_xm_{xy}$, $m_{x\bar{y}}^\star m_{xy} 2_z^\star$	4	2	4	4
	m_x (m_y)	E	$m_xm_y2_z$	$4_zm_xm_{xy}$, $m_x m_y^\star 2_z^\star$	4	2	4	4
	2_z	Reducible	$4_zm_xm_{xy}$	$4_z^\star$, $m_x^\star m_y^\star 2_z$, $m_{x\bar{y}}^\star m_{xy}^\star 2_z$	4	4	2	2
	1	E	$4_zm_xm_{xy}$	4_z, $m_x^\star(2)$, $m_{xy}^\star(2)$, $2_z^\star$	8	8	8	8

† $u = x, y, z, xy, yz, zx, x\bar{y}, y\bar{z}, z\bar{x}, x', x'', y', y''$.

Table 3.4.2.7 (*cont.*)

G	F_1	Γ_η	$N_G(F_1)$	$K_G(F_1, g_{1j})$	n	d_F	n_e	n_a
$\mathbf{\bar{4}_z 2_x m_{xy}}$	$\bar{4}_z$	A_2	$\bar{4}_z 2_x m_{xy}$	$\bar{4}_z 2_x^\star m_{xy}^\star$	2	2	0	1
	$m_{x\bar{y}} m_{xy} 2_z$	B_2	$\bar{4}_z 2_x m_{xy}$	$\bar{4}_z^\star 2_x^\star m_{xy}$	2	2	2	2
	$2_x 2_y 2_z$	B_1	$\bar{4}_z 2_x m_{xy}$	$\bar{4}_z^\star 2_x m_{xy}^\star$	2	2	0	2
	m_{xy} $(m_{x\bar{y}})$	E	$m_{x\bar{y}} m_{xy} 2_z$	$\bar{4}_z 2_x m_{xy}$, $m_{x\bar{y}}^\star m_{xy} 2_z^\star$	4	2	4	4
	2_z	Reducible	$\bar{4}_z 2_x m_{xy}$	$\bar{4}_z^\star$, $m_{x\bar{y}}^\star m_{xy}^\star 2_z$, $2_x^\star 2_y^\star 2_z$	4	4	2	2
	2_x (2_y)	E	$2_x 2_y 2_z$	$\bar{4}_z 2_x m_{xy}$, $2_x 2_y^\star 2_z^\star$	4	2	4	4
	1	E	$\bar{4}_z 2_x m_{xy}$	$\bar{4}_z$, $m_{xy}^\star(2)$, $2_z^\star$, $2_x^\star(2)$	8	8	8	8
$\bar{4}_z m_x 2_{xy}$	$\bar{4}_z$	A_2	$\bar{4}_z m_x 2_{xy}$	$\bar{4}_z m_x^\star 2_{xy}^\star$	2	2	0	1
	$m_x m_y 2_z$	B_2	$\bar{4}_z m_x 2_{xy}$	$\bar{4}_z^\star m_x 2_{xy}^\star$	2	2	2	2
	$2_{x\bar{y}} 2_{xy} 2_z$	B_1	$\bar{4}_z m_x 2_{xy}$	$\bar{4}_z^\star m_x^\star 2_{xy}$	2	2	0	2
	m_x (m_y)	E	$m_x m_y 2_z$	$\bar{4}_z m_x 2_{xy}$, $m_x m_y^\star 2_z^\star$	4	2	4	4
	2_{xy} $(2_{x\bar{y}})$	E	$2_{x\bar{y}} 2_{xy} 2_z$	$\bar{4}_z m_x 2_{xy}$, $2_{x\bar{y}}^\star 2_{xy} 2_z^\star$	4	2	4	4
	2_z	Reducible	$\bar{4}_z m_x 2_{xy}$	$\bar{4}_z^\star$, $m_x^\star m_y^\star 2_z$, $2_{x\bar{y}}^\star 2_{xy}^\star 2_z$	4	4	2	2
	1	E	$\bar{4}_z m_x 2_{xy}$	$\bar{4}_z$, $m_x^\star(2)$, $2_{xy}^\star(2)$, $2_z^\star$	8	8	8	8
$\mathbf{4_z/m_z m_x m_{xy}}$	$\bar{4}_z m_x 2_{xy}$	B_{2u}	$4_z/m_z m_x m_{xy}$	$4_z^\star/m_z^\star m_x m_{xy}^\star$	2	2	0	1
	$\bar{4}_z 2_x m_{xy}$	B_{1u}	$4_z/m_z m_x m_{xy}$	$4_z^\star/m_z^\star m_x^\star m_{xy}$	2	2	0	1
	$4_z m_x m_{xy}$	A_{2u}	$4_z/m_z m_x m_{xy}$	$4_z^\star/m_z^\star m_x m_{xy}$	2	2	2	1
	$4_z 2_x 2_{xy}$	A_{1u}	$4_z/m_z m_x m_{xy}$	$4_z^\star/m_z^\star m_x^\star m_{xy}$	2	2	0	1
	$4_z/m_z$	A_{2g}	$4_z/m_z m_x m_{xy}$	$4_z^\star/m_z m_x^\star m_{xy}^\star$	2	2	0	1
	$\bar{4}_z$	Reducible	$4_z/m_z m_x m_{xy}$	$\bar{4}_z 2_x^\star m_{xy}^\star$, $\bar{4}_z m_x^\star 2_{xy}^\star$, $4_z^\star/m_z^\star$	4	4	0	1
	4_z	Reducible	$4_z/m_z m_x m_{xy}$	$4_z m_x^\star m_{xy}^\star$, $4_z 2_x^\star 2_{xy}^\star$, $4_z/m_z^\star$	4	4	2	1
	$m_{x\bar{y}} m_{xy} m_z$	B_{2g}	$4_z/m_z m_x m_{xy}$	$4_z^\star/m_z m_x^\star m_{xy}$	2	2	0	2
	$m_x m_y m_z$	B_{1g}	$m_x m_y m_z$	$4_z^\star/m_z m_x m_{xy}^\star$	2	2	0	2
	$2_{x\bar{y}} m_{xy} m_z$ $(m_{x\bar{y}} 2_{xy} m_z)$	E_u	$m_{x\bar{y}} m_{xy} m_z$	$4_z/m_z m_x m_{xy}$, $m_{x\bar{y}}^\star m_{xy} m_z$	4	2	4	2
	$2_x m_y m_z$ $(m_x 2_y m_z)$	E_u	$m_x m_y m_z$	$4_z/m_z m_x m_{xy}$, $m_x^\star m_y m_z$	4	2	4	2
	$m_{x\bar{y}} m_{xy} 2_z$	Reducible	$4_z/m_z m_x m_{xy}$	$\bar{4}_z^\star 2_x^\star m_{xy}$, $4_z^\star m_x^\star m_{xy}$, $m_{x\bar{y}} m_{xy} m_z^\star$	4	4	2	2
	$m_x m_y 2_z$	Reducible	$4_z/m_z m_x m_{xy}$	$\bar{4}_z^\star m_x 2_{xy}^\star$, $4_z^\star m_x m_{xy}^\star$, $m_x m_y m_z^\star$	4	4	2	2
	$2_{x\bar{y}} 2_{xy} 2_z$	Reducible	$4_z/m_z m_x m_{xy}$	$\bar{4}_z^\star m_x^\star 2_{xy}$, $4_z^\star 2_x^\star 2_{xy}$, $m_{x\bar{y}}^\star m_{xy}^\star m_z^\star$	4	4	0	2
	$2_x 2_y 2_z$	Reducible	$4_z/m_z m_x m_{xy}$	$\bar{4}_z^\star 2_x m_{xy}^\star$, $4_z^\star 2_x 2_{xy}^\star$, $m_x^\star m_y^\star m_z^\star$	4	4	0	2
	$2_{xy}/m_{xy}$ $(2_{x\bar{y}}/m_{x\bar{y}})$	E_g	$m_{x\bar{y}} m_{xy} m_z$	$4_z/m_z m_x m_{xy}$, $m_{x\bar{y}}^\star m_{xy} m_z^\star$	4	2	0	4
	$2_z/m_z$	Reducible	$4_z/m_z m_x m_{xy}$	$4_z^\star/m_z$, $m_{x\bar{y}}^\star m_{xy}^\star m_z$, $m_x^\star m_y^\star m_z$	4	4	0	4
	$2_x/m_x$ $(2_y/m_y)$	E_g	$m_x m_y m_z$	$4_z/m_z m_x m_{xy}$, $m_x m_y^\star m_z^\star$	4	2	0	4
	$m_{xy}(m_{x\bar{y}})$	Reducible	$m_{x\bar{y}} m_{xy} m_z$	$\bar{4}_z 2_x m_{xy}$, $4_z m_x m_{xy}$, $2_{x\bar{y}}^\star m_{xy} m_z^\star$, $m_{x\bar{y}}^\star m_{xy} 2_z^\star$, $2_{xy}^\star/m_{xy}$	8	4	8	4
	m_z	E_u	$4_z/m_z m_x m_{xy}$	$4_z/m_z$, $2_{x\bar{y}}^\star m_{xy}^\star m_z(2)$, $2_x^\star m_y^\star m_z(2)$, $2_z^\star/m_z$	8	8	8	4
	m_x (m_y)	Reducible	$m_x m_y m_z$	$\bar{4}_z m_x 2_{xy}$, $4_z m_x m_{xy}$, $m_x m_y^\star 2_z^\star$, $m_x 2_y^\star m_z^\star$, $2_x^\star/m_x$	8	4	8	4
	2_{xy} $(2_{x\bar{y}})$	Reducible	$m_{x\bar{y}} m_{xy} m_z$	$\bar{4}_z m_x 2_{xy}$, $4_z 2_x 2_{xy}$, $m_{x\bar{y}}^\star 2_{xy} m_z^\star$, $2_{x\bar{y}}^\star 2_{xy} 2_z^\star$, $2_{xy}/m_{xy}^\star$	8	4	8	4
	2_z	Reducible	$4_z/m_z m_x m_{xy}$	$\bar{4}_z^\star$, $4_z^\star$, $m_x^\star m_y^\star 2_z$, $m_{x\bar{y}}^\star m_{xy}^\star 2_z$, $2_x^\star 2_y^\star 2_z$, $2_{x\bar{y}}^\star 2_{xy}^\star 2_z$, $2_z/m_z^\star$	8	8	2	4
	2_x (2_y)	Reducible	$m_x m_y m_z$	$\bar{4}_z 2_x m_{xy}$, $4_z 2_x 2_{xy}$, $2_x m_y^\star m_z^\star$, $2_x 2_y^\star 2_z^\star$, $2_x/m_x^\star$	8	4	4	4
	$\bar{1}$	E_g	$4_z/m_z m_x m_{xy}$	$4_z/m_z$, $2_{xy}^\star/m_{xy}^\star(2)$, $2_z^\star/m_z^\star$, $2_x^\star/m_x^\star(2)$	8	8	0	8
	1	Reducible	$4_z/m_z m_x m_{xy}$	$\bar{4}_z$, 4_z, $m_{xy}^\star(2)$, $m_z^\star$, $m_x^\star(2)$, $2_{xy}^\star(2)$, $2_z^\star$, $2_x^\star(2)$, $\bar{1}^\star$	16	16	16	8
$\mathbf{3_z}$	1	E	3_z	3_z	3	3	3	3
$\mathbf{\bar{3}_z}$	3_z	A_u	$\bar{3}_z$	$\bar{3}_z^\star$	2	2	2	1
	$\bar{1}$	E_g	$\bar{3}_z$	$\bar{3}_z$	3	3	0	3
	1	E_u	$\bar{3}_z$	$\bar{3}_z$, 3_z, $\bar{1}^\star$	6	6	6	3
$\mathbf{3_z 2_x}$	3_z	A_2	$3_z 2_x$	$3_z 2_x^\star$	2	2	2	1
	2_x $(2_{x'}, 2_{x''})$	E	2_x	$3_z 2_x$	3	1	3	3
	1	E	$3_z 2_x$	3_z, $2_x^\star(3)$	6	6	6	6
$3_z 2_y$	3_z	A_2	$3_z 2_y$	$3_z 2_y^\star$	2	2	2	1
	2_y $(2_{y'}, 2_{y''})$	E	2_y	$3_z 2_y$	3	1	3	3
	1	E	$3_z 2_y$	3_z, $2_y^\star(3)$	6	6	6	6
$\mathbf{3_z m_x}$	3_z	A_2	$3_z m_x$	$3_z m_x^\star$	2	2	1	1
	m_x $(m_{x'}, m_{x''})$	E	m_x	$3_z m_x$	3	1	3	3
	1	E	$3_z m_x$	3_z, $m_x^\star(3)$	6	6	6	6
$3_z m_y$	3_z	A_2	$3_z m_y$	$3_z m_y^\star$	2	2	1	1
	m_y $(m_{y'}, m_{y''})$	E	m_y	$3_z m_y$	3	1	3	3
	1	E	$3_z m_y$	3_z, $m_y^\star(3)$	6	6	6	6

Table 3.4.2.7 (*cont.*)

G	F_1	Γ_η	$N_G(F_1)$	$K_G(F_1, g_{1j})$	n	d_F	n_e	n_a
$\bar{3}_z m_x$	$3_z m_x$	A_{2u}	$\bar{3}_z m_x$	$\bar{3}^\star_z m_x$	2	2	2	1
	$3_z 2_x$	A_{1u}	$\bar{3}_z m_x$	$\bar{3}^\star_z m^\star_x$	2	2	0	1
	$\bar{3}_z$	A_{2g}	$\bar{3}_z m_x$	$\bar{3}_z m^\star_x$	2	2	0	1
	3_z	Reducible	$\bar{3}_z m_x$	$3_z m^\star_x$, $3_z 2^\star_x$, $\bar{3}^\star_z$	4	4	2	1
	$2_x/m_x$ $(2_{x'}/m_{x'}, 2_{x''}/m_{x''})$	E_g	$2_x/m_x$	$\bar{3}_z m_x$	3	1	0	3
	m_x $(m_{x'}, m_{x''})$	E_u	$2_x/m_x$	$\bar{3}_z m_x$, $3_z m_x$, $2^\star_x/m_x(3)$	6	2	6	3
	2_x $(2_{x'}, 2_{x''})$	E_u	$2_x/m_x$	$\bar{3}_z m_x$, $3_z 2_x$, $2_x/m^\star_x(3)$	6	2	6	3
	$\bar{1}$	E_g	$\bar{3}_z m_x$	$\bar{3}_z$, $2^\star_x/m^\star_x(3)$	6	6	0	6
	1	E_u	$\bar{3}_z m_x$	$\bar{3}_z$, 3_z, $m^\star_x(3)$, $2^\star_x(3)$, $\bar{1}^\star$	12	12	12	6
$\bar{3}_z m_y$	$3_z m_y$	A_{2u}	$\bar{3}_z m_y$	$\bar{3}^\star_z m_y$	2	2	2	1
	$3_z 2_y$	A_{1u}	$\bar{3}_z m_y$	$\bar{3}^\star_z m^\star_y$	2	2	0	1
	$\bar{3}_z$	A_{2g}	$\bar{3}_z m_y$	$\bar{3}_z m^\star_y$	2	2	0	1
	3_z	Reducible	$\bar{3}_z m_y$	$3_z m^\star_y$, $3_z 2^\star_y$, $\bar{3}^\star_z$	4	4	0	1
	$2_y/m_y$ $(2_{y'}/m_{y'}, 2_{y''}/m_{y''})$	E_g	$2_y/m_y$	$\bar{3}_z m_y$	3	1	2	1
	m_y $(m_{y'}, m_{y''})$	E_u	$2_y/m_y$	$\bar{3}_z m_y$, $3_z m_y$, $2^\star_y/m_y(3)$	6	2	0	3
	2_y $(2_{y'}, 2_{y''})$	E_u	$2_y/m_y$	$\bar{3}_z m_y$, $3_z 2_y$, $2_y/m^\star_y(3)$	6	2	6	3
	$\bar{1}$	E_g	$\bar{3}_z m_y$	$\bar{3}_z$, $2^\star_y/m^\star_y(3)$	6	6	0	3
	1	E_u	$\bar{3}_z m_y$	$\bar{3}_z$, 3_z, $m^\star_y(3)$, $2^\star_y(3)$, $\bar{1}^\star$	12	12	12	6
6_z	3_z	B	6_z	$6^\star_z$	2	2	1	1
	2_z	E_2	6_z	6_z	3	3	1	3
	1	E_1	6_z	6_z, 3_z, $2^\star_z$	6	6	6	6
$\bar{6}_z$	3_z	A''	$\bar{6}_z$	$\bar{6}^\star_z$	2	2	2	1
	m_z	E'	$\bar{6}_z$	$\bar{6}_z$	3	2	3	3
	1	E''	$\bar{6}_z$	$\bar{6}_z$, 3_z, $m^\star_z$	6	6	6	6
$6_z/m_z$	$\bar{6}_z$	B_u	$6_z/m_z$	$6^\star_z/m_z$	2	2	0	1
	6_z	A_u	$6_z/m_z$	$6_z/m^\star_z$	2	2	2	1
	$\bar{3}_z$	B_g	$6_z/m_z$	$6^\star_z/m^\star_z$	2	2	0	1
	3_z	Reducible	$6_z/m_z$	$\bar{6}^\star_z$, $6^\star_z$, $\bar{3}^\star_z$	4	4	2	1
	$2_z/m_z$	E_{2g}	$6_z/m_z$	$6_z/m_z$	3	3	0	3
	m_z	E_{1u}	$6_z/m_z$	$6_z/m_z$, $\bar{6}_z$, $2^\star_z/m_z$	6	6	6	3
	2_z	E_{2u}	$6_z/m_z$	$6_z/m_z$, 6_z, $2_z/m^\star_z$	6	6	2	3
	$\bar{1}$	E_{1g}	$6_z/m_z$	$6_z/m_z$, $\bar{3}_z$, $2^\star_z/m^\star_z$	6	6	0	6
	1	Reducible	$6_z/m_z$	$\bar{6}_z$, 6_z, $\bar{3}_z$, 3_z, $m^\star_z$, $2^\star_z$, $\bar{1}^\star$	12	12	12	6
$6_z 2_x 2_y$	6_z	A_2	$6_z 2_x 2_y$	$6_z 2^\star_x 2^\star_y$	2	2	2	1
	$3_z 2_x$	B_1	$6_z 2_x 2_y$	$6^\star_z 2_x 2^\star_y$	2	2	0	1
	$3_z 2_y$	B_2	$6_z 2_x 2_y$	$6^\star_z 2^\star_x 2_y$	2	2	0	1
	3_z	Reducible	$6_z 2_x 2_y$	$6^\star_z$, $3_z 2^\star_x$, $3_z 2^\star_y$	4	4	2	1
	$2_x 2_y 2_z$ $(2_{x'} 2_{y'} 2_z, 2_{x''} 2_{y''} 2_z)$	E_2	$2_x 2_y 2_z$	$6_z 2_x 2_y$	3	1	0	3
	2_z	E_2	$6_z 2_x 2_y$	6_z, $2^\star_x 2^\star_y 2_z(3)$	6	6	2	6
	2_x $(2_{x'}, 2_{x''})$	E_1	$2_x 2_y 2_z$	$6_z 2_x 2_y$, $3_z 2_x$, $2_x 2^\star_y 2^\star_z$	6	2	6	6
	2_y $(2_{y'}, 2_{y''})$	E_1	$2_x 2_y 2_z$	$6_z 2_x 2_y$, $3_z 2_y$, $2^\star_x 2_y 2^\star_z$	6	2	6	6
	1	E_1	$6_z 2_x 2_y$	6_z, 3_z, $2^\star_z$, $2^\star_x(3)$, $2^\star_y(3)$	12	12	12	12
$6_z m_x m_y$	6_z	A_2	$6_z m_x m_y$	$6_z m^\star_x m^\star_y$	2	2	1	1
	$3_z m_x$	B_2	$6_z m_x m_y$	$6^\star_z m_x m^\star_y$	2	2	1	1
	$3_z m_y$	B_1	$6_z m_x m_y$	$6^\star_z m^\star_x m_y$	2	2	1	1
	3_z	Reducible	$6_z m_x m_y$	$6^\star_z$, $3_z m^\star_x$, $3_z m^\star_y$	4	4	1	1
	$m_x m_y 2_z$ $(m_{x'} m_{y'} 2_z, m_{x''} m_{y''} 2_z)$	E_2	$m_x m_y 2_z$	$6_z m_x m_y$	3	1	1	3
	m_x $(m_{x'}, m_{x''})$	E_1	$m_x m_y 2_z$	$6_z m_x m_y$, $3_z m_x$, $m_x m^\star_y 2^\star_z$	6	2	6	6
	m_y $(m_{y'}, m_{y''})$	E_1	$m_x m_y 2_z$	$6_z m_x m_y$, $3_z m_y$, $m^\star_x m_y 2^\star_z$	6	2	6	6
	2_z	E_2	$6_z m_x m_y$	6_z, $m^\star_x m^\star_y 2_z(3)$	6	6	1	6
	1	E_1	$6_z m_x m_y$	6_z, 3_z, $2^\star_z$, $m^\star_x(3)$, $m^\star_y(3)$	12	12	12	12
$\bar{6}_z m_x 2_y$	$\bar{6}_z$	$A_2{}'$	$\bar{6}_z m_x 2_y$	$\bar{6}_z m^\star_x 2^\star_y$	2	2	0	1
	$3_z m_x$	$A_2{}''$	$\bar{6}_z m_x 2_y$	$\bar{6}^\star_z m_x 2^\star_y$	2	2	2	1
	$3_z 2_y$	$A_1{}'$	$\bar{6}_z m_x 2_y$	$\bar{6}^\star_z m^\star_x 2_y$	2	2	0	1
	3_z	Reducible	$\bar{6}_z m_x 2_y$	$\bar{6}^\star_z$, $3_z m^\star_x$, $3_z 2^\star_y$	4	4	2	1
	$m_x 2_y m_z$ $(m_{x'} 2_{y'} m_z, m_{x''} 2_{y''} m_z)$	E'	$m_x 2_y m_z$	$\bar{6}_z m_x 2_y$	3	1	3	3
	m_z	E'	$\bar{6}_z m_x 2_y$	$\bar{6}_z$, $m^\star_x 2^\star_y m_z(3)$	6	6	6	6
	m_x $(m_{x'}, m_{x''})$	E''	$m_y 2_y m_z$	$\bar{6}_z m_x 2_y$, $3_z m_x$, $m_x 2^\star_y m^\star_z$	6	2	6	6
	2_y $(2_{y'}, 2_{y''})$	E''	$m_x 2_y m_z$	$\bar{6}_z m_x 2_y$, $3_z 2_y$, $m^\star_x 2_y m^\star_z$	6	2	3	6
	1	E''	$\bar{6}_z m_x 2_y$	$\bar{6}_z$, 3_z, $m^\star_z$, $m^\star_x(3)$, $2^\star_y(3)$	12	12	12	12

Table 3.4.2.7 (*cont.*)

G	F_1	Γ_η	$N_G(F_1)$	$K_G(F_1, g_{1j})$	n	d_F	n_e	n_a
$\bar{6}_z2_xm_y$	$\bar{6}_z$	A_2'	$\bar{6}_z2_xm_y$	$\bar{6}_z2^{\star}_xm^{\star}_y$	2	2	0	1
	3_zm_y	A_2'	$\bar{6}_z2_xm_y$	$\bar{6}^{\star}_z2^{\star}_xm_y$	2	2	2	1
	3_z2_x	A_1''	$\bar{6}_z2_xm_y$	$\bar{6}^{\star}_z2_xm^{\star}_y$	2	2	0	1
	3_z	Reducible	$\bar{6}_z2_xm_y$	$\bar{6}^{\star}_z$, $3_zm^{\star}_y$, $3_z2^{\star}_x$	4	4	2	1
	$2_xm_ym_z$ ($2_{x'}m_{y'}m_z$, $2_{x''}m_{y''}m_z$)	E'	$m_x2_ym_z$	$\bar{6}_z2_xm_y$	3	1	3	3
	m_z	E'	$\bar{6}_z2_xm_y$	$\bar{6}_z$, $2^{\star}_xm^{\star}_ym_z(3)$	6	6	6	6
	m_y ($m_{y'}$, $m_{y''}$)	E''	$m_x2_ym_z$	$\bar{6}_z2_xm_y$, 3_zm_y, $2^{\star}_xm_ym^{\star}_z$	6	2	6	6
	2_x ($2_{x'}$, $2_{x''}$)	E''	$m_x2_ym_z$	$\bar{6}_z2_xm_y$, 3_z2_x, $2_xm^{\star}_ym^{\star}_z$	6	2	3	6
	1	E''	$\bar{6}_z2_xm_y$	$\bar{6}_z$, 3_z, $m^{\star}_z$, $m^{\star}_y(3)$, $2^{\star}_x(3)$	12	12	12	12
$\mathbf{6_z/m_zm_xm_y}$	$\bar{6}_zm_x2_y$	B_{2u}	$6_z/m_zm_xm_y$	$6^{\star}_z/m_zm_xm^{\star}_y$	2	2	0	1
	$\bar{6}_z2_xm_y$	B_{1u}	$6_z/m_zm_xm_y$	$6^{\star}_z/m_zm^{\star}_xm_y$	2	2	0	1
	$6_zm_xm_y$	A_{2u}	$6_z/m_zm_xm_y$	$6_z/m^{\star}_zm_xm_y$	2	2	2	1
	$6_z2_x2_y$	A_{1u}	$6_z/m_zm_xm_y$	$6_z/m^{\star}_zm^{\star}_xm^{\star}_y$	2	2	0	1
	$6_z/m_z$	A_{2g}	$6_z/m_zm_xm_y$	$6_z/m_zm^{\star}_xm^{\star}_y$	2	2	0	1
	$\bar{6}_z$	Reducible	$6_z/m_zm_xm_y$	$\bar{6}_zm^{\star}_x2^{\star}_y$, $\bar{6}_z2^{\star}_xm^{\star}_y$, $6^{\star}_z/m_z$	4	4	0	1
	6_z	Reducible	$6_z/m_zm_xm_y$	$6_zm^{\star}_xm^{\star}_y$, $6_z2^{\star}_x2^{\star}_y$, $6_z/m^{\star}_z$	4	4	2	1
	$\bar{3}_zm_x$	B_{1g}	$6_z/m_zm_xm_y$	$6^{\star}_z/m^{\star}_zm_xm^{\star}_y$	2	2	0	1
	$\bar{3}_zm_y$	B_{2g}	$6_z/m_zm_xm_y$	$6^{\star}_z/m^{\star}_zm^{\star}_xm_y$	2	2	0	1
	3_zm_x	Reducible	$6_z/m_zm_xm_y$	$\bar{6}^{\star}_zm_x2^{\star}_y$, $6^{\star}_zm_xm^{\star}_y$, $\bar{3}^{\star}_zm_x$	4	4	2	1
	3_zm_y	Reducible	$6_z/m_zm_xm_y$	$\bar{6}^{\star}_z2^{\star}_xm_y$, $6^{\star}_zm^{\star}_xm_y$, $\bar{3}^{\star}_zm_y$	4	4	2	1
	3_z2_x	Reducible	$6_z/m_zm_xm_y$	$\bar{6}^{\star}_z2_xm^{\star}_y$, $6^{\star}_z2_x2^{\star}_y$, $\bar{3}^{\star}_zm^{\star}_x$	4	4	0	1
	3_z2_y	Reducible	$6_z/m_zm_xm_y$	$\bar{6}^{\star}_zm^{\star}_x2_y$, $6^{\star}_z2^{\star}_x2_y$, $\bar{3}^{\star}_zm^{\star}_y$	4	4	0	1
	$\bar{3}_z$	Reducible	$6_z/m_zm_xm_y$	$6^{\star}_z/m^{\star}_z$, $\bar{3}_zm^{\star}_x$, $\bar{3}_zm^{\star}_y$	4	4	0	1
	3_z	Reducible	$6_z/m_zm_xm_y$	$\bar{6}^{\star}_z$, $6^{\star}_z$, $3_zm^{\star}_x$, $3_zm^{\star}_y$, $3_z2^{\star}_x$, $3_z2^{\star}_y$, $\bar{3}^{\star}_z$	8	8	2	1
	$m_xm_ym_z$ ($m_{x'}m_{y'}m_z$, $m_{x''}m_{y''}m_z$)	E_{2g}	$m_xm_ym_z$	$6_z/m_zm_xm_y$	3	1	0	3
	$m_xm_y2_z$ ($m_{x'}m_{y'}2_z$, $m_{x''}m_{y''}2_z$)	E_{2u}	$m_xm_ym_z$	$6_z/m_zm_xm_y$, $6_zm_xm_y$, $m_xm_ym^{\star}_z$	6	2	2	3
	$2_xm_ym_z$ ($2_{x'}m_{y'}m_z$, $2_{x''}m_{y''}m_z$)	E_{1u}	$m_xm_ym_z$	$6_z/m_zm_xm_y$, $\bar{6}_z2_xm_y$, $m^{\star}_xm_ym_z$	6	2	6	3
	$m_x2_ym_z$ ($m_{x'}2_{y'}m_z$, $m_{x''}2_{y''}m_z$)	E_{1u}	$m_xm_ym_z$	$6_z/m_zm_xm_y$, $\bar{6}_zm_x2_y$, $m_xm^{\star}_ym_z$	6	2	6	3
	$2_x2_y2_z$ ($2_{x'}2_{y'}2_z$, $2_{x''}2_{y''}2_z$)	E_{2u}	$m_xm_ym_z$	$6_z/m_zm_xm_y$, $6_z2_x2_y$, $m^{\star}_xm^{\star}_ym^{\star}_z$	6	6	0	3
	$2_z/m_z$	E_{2g}	$6_z/m_zm_xm_y$	$6_z/m_z$, $m^{\star}_xm^{\star}_ym_z(3)$	6	6	0	6
	$2_x/m_x$ ($2_{x'}/m_{x'}$, $2_{x''}/m_{x''}$)	E_{1g}	$m_xm_ym_z$	$6_z/m_zm_xm_y$, $\bar{3}_zm_x$, $m_xm^{\star}_ym^{\star}_z$	6	2	0	6
	$2_y/m_y$ ($2_{y'}/m_{y'}$, $2_{y''}/m_{y''}$)	E_{1g}	$m_xm_ym_z$	$6_z/m_zm_xm_y$, $\bar{3}m_y$, $m^{\star}_xm_ym^{\star}_z$	6	2	0	6
	m_z	E_{1u}	$6_z/m_zm_xm_y$	$6_z/m_z$, $\bar{6}_z$, $2^{\star}_xm^{\star}_ym_z$, $m^{\star}_x2^{\star}_ym_z$, $2^{\star}_z/m_z$	12	12	12	6
	m_x ($m_{x'}$, $m_{x''}$)	Reducible	$m_xm_ym_z$	$\bar{6}_zm_x2_y$, $6_zm_xm_y$, $\bar{3}_zm_x$, 3_zm_x, $m_xm^{\star}_y2^{\star}_z$, $m_x2^{\star}_ym^{\star}_z$, $2^{\star}_x/m_x$	12	4	12	6
	m_y ($m_{y'}$, $m_{y''}$)	Reducible	$m_xm_ym_z$	$\bar{6}_z2_xm_y$, $6_zm_xm_y$, $\bar{3}_zm_y$, 3_zm_y, $m^{\star}_xm_y2^{\star}_z$, $2^{\star}_xm_ym^{\star}_z$, $2^{\star}_y/m_y$	12	4	12	6
	2_z	E_{2u}	$6_z/m_zm_xm_y$	$6_z/m_z$, 6_z, $m^{\star}_xm^{\star}_y2_z(3)$, $2^{\star}_x2^{\star}_y2_z(3)$, $2_z/m^{\star}_z$	12	12	2	6
	2_x ($2_{x'}$, $2_{x''}$)	Reducible	$m_xm_ym_z$	$\bar{6}_z2_xm_y$, $6_z2_x2_y$, $\bar{3}_zm_x$, 3_z2_x, $2_xm^{\star}_ym^{\star}_z$, $2_x2^{\star}_y2^{\star}_z$, $2_x/m^{\star}_x$	12	4	6	6
	2_y ($2_{y'}$, $2_{y''}$)	Reducible	$m_xm_ym_z$	$\bar{6}_zm_x2_y$, $6_z2_x2_y$, $\bar{3}_zm_y$, 3_z2_y, $m^{\star}_x2_ym^{\star}_z$, $2^{\star}_x2_y2^{\star}_z$, $2_y/m^{\star}_y$	12	4	6	6
	$\bar{1}$	E_{1g}	$6_z/m_zm_xm_y$	$6_z/m_z$, $\bar{3}_z$, $2^{\star}_z/m^{\star}_z$, $2^{\star}_x/m^{\star}_x(3)$, $2^{\star}_y/m^{\star}_y(3)$	12	12	0	12
	1	Reducible	$6_z/m_zm_xm_y$	$\bar{6}_z$, 6_z, $\bar{3}_z$, 3_z, $m^{\star}_z$, $m^{\star}_x(3)$, $m^{\star}_y(3)$, $2^{\star}_z$, $2^{\star}_x(3)$, $2^{\star}_y(3)$, $\bar{1}^{\star}$	24	24	24	12
23	3_p (3_q, 3_r, 3_s)	T	3_p	23	4	1	4	4
	$2_x2_y2_z$	E	23	23	3	3	0	3
	2_z (2_x, 2_y)	T	$2_x2_y2_z$	23, $2^{\star}_x2^{\star}_y2_z$	6	2	6	6
	1	T	23	$3_p(4)$, $2^{\star}_z(3)$	12	12	12	12
$\mathbf{m\bar{3}}$	23	A_u	$m\bar{3}$	$m^{\star}\bar{3}^{\star}$	2	2	0	1
	$\bar{3}_p$ ($\bar{3}_q$, $\bar{3}_r$, $\bar{3}_s$)	T_g	$\bar{3}_p$	$m\bar{3}$	4	1	0	4
	3_p (3_q, 3_r, 3_s)	T_u	$\bar{3}_p$	$m\bar{3}$, 23	8	2	8	4
	$m_xm_ym_z$	E_g	$m\bar{3}$	$m\bar{3}$	3	3	0	3
	$m_xm_y2_z$ ($2_xm_ym_z$, $m_x2_ym_z$)	T_u	$m_xm_ym_z$	$m\bar{3}$, $m_xm_ym^{\star}_z$	6	2	6	3
	$2_x2_y2_z$	E_u	$m\bar{3}$	$m\bar{3}$, 23, $m^{\star}_xm^{\star}_ym^{\star}_z$	6	6	0	3
	$2_z/m_z$ ($2_x/m_x$, $2_y/m_y$)	T_g	$m_xm_ym_z$	$m\bar{3}$, $m^{\star}_xm^{\star}_ym_z$	6	2	0	6
	m_z (m_x, m_y)	T_u	$m_xm_ym_z$	$m\bar{3}$, $2^{\star}_xm^{\star}_ym_z$, $m^{\star}_x2^{\star}_ym_z$, $2^{\star}_z/m_z$	12	4	12	6
	2_z (2_x, 2_y)	Reducible	$m_xm_ym_z$	$m\bar{3}$, 23, $m^{\star}_xm^{\star}_y2_z$, $2^{\star}_x2^{\star}_y2_z$, $2_z/m^{\star}_z$	12	4	6	6
	$\bar{1}$	T_g	$m\bar{3}$	$\bar{3}_p(4)$, $2^{\star}_z/m^{\star}_z(3)$	12	12	0	12
	1	T_u	$m\bar{3}$	$\bar{3}_p(4)$, $3_p(4)$, $m^{\star}_z(3)$, $2^{\star}_z(3)$, $\bar{1}^{\star}$	24	24	24	12

Table 3.4.2.7 (*cont.*)

G	F_1	Γ_η	$N_G(F_1)$	$K_G(F_1, g_{1j})$	n	d_F	n_e	n_a
432	23	A_2	432	$4^{\star}32^{\star}$	2	2	0	1
	$3_p2_{x\bar{y}}$ $(3_q2_{x\bar{y}}, 3_r2_{xy}, 3_s2_{xy})$	T_2	$3_p2_{x\bar{y}}$	432	4	1	0	4
	3_p $(3_q, 3_r, 3_s)$	T_1	$3_p2_{x\bar{y}}$	23, $3_p2^{\star}_{x\bar{y}}$	8	2	8	4
	$4_z2_x2_{xy}$ $(4_x2_y2_{yz}, 4_y2_z2_{xz})$	E	$4_z2_x2_{xy}$	432	3	1	0	3
	4_z $(4_x, 4_y)$	T_1	$4_z2_x2_{xy}$	432, $4_z2^{\star}_x2^{\star}_{xy}$	6	2	6	3
	$2_x2_y2_z$	E	432	23, $4^{\star}_z2_x2^{\star}_{xy}$	6	6	0	6
	$2_{x\bar{y}}2_{xy}2_z$ $(2_{y\bar{z}}2_{yz}2_x, 2_{z\bar{x}}2_{zx}2_y)$	T_2	$4_z2_x2_{xy}$	432, $4^{\star}_z2^{\star}_x2_{xy}$	6	2	0	6
	2_z $(2_x, 2_y)$	Reducible	$4_z2_x2_{xy}$	23, $4_y2_z2_{xy}$, $4^{\star}_z$, $2^{\star}_{x\bar{y}}2^{\star}_{xy}2_z$, $2^{\star}_x2^{\star}_y2_z$	12	4	6	12
	2_{xy} $(2_{yz}, 2_{zx}, 2_{x\bar{y}}, 2_{y\bar{z}}, 2_{z\bar{x}})$	T_1, T_2	$2_{x\bar{y}}2_{xy}2_z$	432, 3_r2_{xy}, 3_s2_{xy}, $4_z2_x2_{xy}$, $2_{x\bar{y}}2^{\star}_{xy}2^{\star}_z$	12	2	12	12
	1	T_1, T_2	432	$3_p(4)$, $4_z(3)$, $2^{\star}_z(3)$, $2^{\star}_{xy}(6)$	24	24	24	24
$\bar{4}3m$	23	A_2	$\bar{4}3m$	$\bar{4}^{\star}3m^{\star}$	2	2	0	1
	$3_pm_{x\bar{y}}$ $(3_qm_{x\bar{y}}, 3_rm_{xy}, 3_sm_{xy})$	T_2	$3_pm_{x\bar{y}}$	$\bar{4}3m$	4	1	4	4
	3_p $(3_q, 3_r, 3_s)$	T_1	$3_pm_{x\bar{y}}$	$\bar{4}3m$, 23, $3_pm^{\star}_{x\bar{y}}$	8	2	4	4
	$\bar{4}_z2_xm_{xy}$ $(\bar{4}_x2_ym_{yz}, \bar{4}_y2_zm_{zx})$	E	$\bar{4}_z2_xm_{x\bar{y}}$	$\bar{4}3m$	3	1	0	3
	$\bar{4}_z$ $(\bar{4}_x, \bar{4}_y)$	T_1	$\bar{4}_z2_xm_{x\bar{y}}$	$\bar{4}3m$, $\bar{4}_z2^{\star}_xm^{\star}_{xy}$	6	2	0	3
	$m_{x\bar{y}}m_{xy}2_z$ $(m_{y\bar{z}}m_{yz}2_x, m_{z\bar{x}}m_{zx}2_y)$	T_2	$\bar{4}_z2_xm_{x\bar{y}}$	$\bar{4}3m$, $\bar{4}^{\star}_z2^{\star}_xm_{xy}$	6	2	6	6
	$2_x2_y2_z$	E	$\bar{4}3m$	23, $\bar{4}^{\star}_z2_xm^{\star}_{xy}$	6	6	0	6
	m_{xy} $(m_{yz}, m_{zx}, m_{x\bar{y}}, m_{y\bar{z}}, m_{z\bar{x}})$	T_1, T_2	$m_{x\bar{y}}m_{xy}2_z$	$\bar{4}3m$, 3_rm_{xy}, 3_sm_{xy}, $\bar{4}_z2_xm_{xy}$, $m^{\star}_{x\bar{y}}m_{xy}2^{\star}_z$	12	2	12	12
	2_z $(2_x, 2_y)$	Reducible	$\bar{4}_z2_xm_{xy}$	23, $\bar{4}^{\star}_z$, $4^{\star}_z$, $m^{\star}_{x\bar{y}}m^{\star}_{xy}2_z$, $2^{\star}_x2^{\star}_y2_z$	12	4	6	12
	1	T_1, T_2	$\bar{4}3m$	$3_p(4)$, $\bar{4}_z(3)$, $m^{\star}_{xy}(6)$, $2^{\star}_z(3)$	24	24	24	24
$m\bar{3}m$	$\bar{4}3m$	A_{2u}	$m\bar{3}m$	$m^{\star}\bar{3}^{\star}m$	2	2	0	1
	432	A_{1u}	$m\bar{3}m$	$m^{\star}\bar{3}^{\star}m^{\star}$	2	2	0	1
	$m\bar{3}$	A_{2g}	$m\bar{3}m$	$m\bar{3}m^{\star}$	2	2	0	1
	23	Reducible	$m\bar{3}m$	$\bar{4}^{\star}3m^{\star}$, $4^{\star}32^{\star}$, $m^{\star}_z\bar{3}_p$	4	4	0	1
	$\bar{3}_pm_{x\bar{y}}$ $(\bar{3}_qm_{x\bar{y}}, \bar{3}_rm_{xy}, \bar{3}_sm_{xy})$	T_{2g}	$\bar{3}_pm_{x\bar{y}}$	$m\bar{3}m$	4	1	0	4
	$3_pm_{x\bar{y}}$ $(3_qm_{x\bar{y}}, 3_rm_{xy}, 3_sm_{xy})$	T_{1u}	$\bar{3}_pm_{x\bar{y}}$	$m\bar{3}m$, $\bar{4}3m$, $\bar{3}^{\star}_pm_{x\bar{y}}$	8	2	8	4
	$3_p2_{x\bar{y}}$ $(3_q2_{x\bar{y}}, 3_r2_{xy}, 3_s2_{xy})$	T_{2u}	$\bar{3}_pm_{x\bar{y}}$	$m\bar{3}m$, 432, $\bar{3}^{\star}_pm_{x\bar{y}}$	8	2	0	4
	$\bar{3}_p$ $(\bar{3}_q, \bar{3}_r, \bar{3}_s)$	T_{1g}	$\bar{3}_pm_{x\bar{y}}$	$m\bar{3}m$, $m\bar{3}$, $\bar{3}_pm^{\star}_{x\bar{y}}$	8	2	0	4
	3_p $(3_q, 3_r, 3_s)$	Reducible	$\bar{3}_pm_{x\bar{y}}$	$\bar{4}3m$, 432, $m\bar{3}$, 23, $3_pm^{\star}_{x\bar{y}}$, $3_p2^{\star}_{x\bar{y}}$, $\bar{3}^{\star}_p$	16	4	8	4
	$4_z/m_zm_xm_{xy}$ $(4_x/m_xm_ym_{yz}$, $4_y/m_ym_zm_{zx})$	E_g	$4_z/m_zm_xm_{xy}$	$m\bar{3}m$	3	1	0	3
	$\bar{4}_z2_xm_{xy}$ $(\bar{4}_x2_ym_{yz}, \bar{4}_y2_zm_{zx})$	E_u	$4_z/m_zm_xm_{xy}$	$m\bar{3}m$, $\bar{4}3m$, $4^{\star}_z/m^{\star}_zm^{\star}_xm_{xy}$	6	2	0	3
	$\bar{4}_zm_x2_{xy}$ $(\bar{4}_xm_y2_{yz}, \bar{4}_ym_z2_{zx})$	T_{2u}	$4_z/m_zm_xm_{xy}$	$m\bar{3}m$, $4^{\star}_z/m^{\star}_zm_xm^{\star}_{xy}$	6	2	0	3
	$4_zm_xm_{xy}$ $(4_xm_ym_{yz}, 4_ym_zm_{zx})$	T_{1u}	$4_z/m_zm_xm_{xy}$	$m\bar{3}m$, $4_z/m^{\star}_zm_xm_{xy}$	6	2	6	3
	$4_z2_x2_{xy}$ $(4_x2_y2_{yz}, 4_y2_z2_{zx})$	E_u	$4_z/m_zm_xm_{xy}$	$m\bar{3}m$, 432, $4_z/m^{\star}_zm^{\star}_xm^{\star}_{xy}$	6	2	0	3
	$4_z/m_z$ $(4_x/m_x, 4_y/m_y)$	T_{1g}	$4_z/m_zm_xm_{xy}$	$m\bar{3}m$, $4_z/m_zm^{\star}_xm^{\star}_{xy}$	6	2	0	3
	$\bar{4}_z$ $(\bar{4}_x, \bar{4}_y)$	Reducible	$4_z/m_zm_xm_{xy}$	$m\bar{3}m$, $\bar{4}3m$, $\bar{4}_z2^{\star}_xm^{\star}_{xy}$, $\bar{4}_zm^{\star}_x2^{\star}_{xy}$, $4^{\star}_z/m^{\star}_z$	12	4	0	3
	4_z $(4_x, 4_y)$	Reducible	$4_z/m_zm_xm_{xy}$	$m\bar{3}m$, 432, $4_zm^{\star}_xm^{\star}_{xy}$, $4_z2^{\star}_x2^{\star}_{xy}$, $4_z/m^{\star}_z$	12	4	6	3
	$m_xm_ym_z$	E_g	$m\bar{3}m$	$m\bar{3}$, $4^{\star}_z/m_zm_xm^{\star}_{xy}$	6	6	0	6
	$m_{x\bar{y}}m_{xy}m_z$ $(m_{y\bar{z}}m_{yz}m_x$, $m_{z\bar{x}}m_{zx}m_y)$	T_{2g}	$4_z/m_zm_xm_{xy}$	$m\bar{3}m$, $4^{\star}_z/m_zm_xm^{\star}_{xy}$	6	2	0	6
	$m_xm_y2_z$ $(2_xm_ym_z, m_x2_ym_z)$	Reducible	$4_z/m_zm_xm_{xy}$	$m\bar{3}$, $4_y/m_ym_zm_{zx}$, $\bar{4}^{\star}_zm_x2^{\star}_{xy}$, $4^{\star}_zm_xm^{\star}_{xy}$, $m_xm_ym^{\star}_z$	12	4	6	6
	$m_{x\bar{y}}m_{xy}2_z$ $(m_{y\bar{z}}m_{yz}2_x, m_{z\bar{x}}m_{zx}2_y)$	Reducible	$4_z/m_zm_xm_{xy}$	$m\bar{3}m$, $\bar{4}3m$, $\bar{4}^{\star}_z2^{\star}_xm_{xy}$, $4^{\star}_zm^{\star}_xm_{xy}$, $m_{x\bar{y}}m_{xy}m^{\star}_z$	12	4	6	6
	$m_{x\bar{y}}2_{xy}m_z$ $(m_{y\bar{z}}2_{yz}m_x, m_{z\bar{x}}2_{zx}m_y$, $2_{x\bar{y}}m_{xy}m_z, 2_{y\bar{z}}m_{yz}m_x$, $2_{z\bar{x}}m_{zx}m_y)$	T_{1u}, T_{2u}	$m_{x\bar{y}}m_{xy}m_z$	$m\bar{3}m(m_{zx})$, $m\bar{3}m(2_{zx})$, $4_z/m_zm_xm_{xy}$, $m_{x\bar{y}}m^{\star}_{xy}m_z$	12	2	12	6
	$2_x2_y2_z$	E_u	$m\bar{3}m$	$m\bar{3}$, 23, $\bar{4}^{\star}_z2_xm^{\star}_{xy}$, $4^{\star}_z2_x2^{\star}_{xy}$, $m^{\star}_xm^{\star}_ym^{\star}_z$	12	12	0	6
	$2_{x\bar{y}}2_{xy}2_z$ $(2_{y\bar{z}}2_{yz}2_x, 2_{z\bar{x}}2_{zx}2_y)$	Reducible	$4_z/m_zm_xm_{xy}$	$m\bar{3}m$, 432, $\bar{4}_zm^{\star}_x2_{xy}$, $4^{\star}_z2^{\star}_x2_{xy}$, $m^{\star}_{x\bar{y}}m^{\star}_{xy}m^{\star}_z$	12	4	0	6
	$2_z/m_z$ $(2_x/m_x, 2_y/m_y)$	Reducible	$4_z/m_zm_xm_{x\bar{y}}$	$m\bar{3}$, $4_y/m_ym_zm_{zx}$, $4^{\star}_z/m_z$, $m^{\star}_xm^{\star}_ym_z$, $m^{\star}_{x\bar{y}}m^{\star}_{xy}m_z$	12	4	0	12
	$2_{xy}/m_{xy}$ $(2_{yz}/m_{yz}, 2_{zx}/m_{zx}$, $2_{x\bar{y}}/m_{x\bar{y}}, 2_{y\bar{z}}/m_{y\bar{z}}, 2_{z\bar{x}}/m_{z\bar{x}})$	T_{1g}, T_{2g}	$m_{x\bar{y}}m_{xy}m_z$	$m\bar{3}m$, $\bar{3}_rm_{xy}(2)$, $4_z/m_zm_xm_{xy}$, $m^{\star}_{x\bar{y}}m_{xy}m^{\star}_z$	12	2	0	12
	m_z (m_x, m_y)	T_{1u}, T_{2u}	$4_z/m_zm_xm_{x\bar{y}}$	$m\bar{3}$, $\bar{4}_xm_z2_{yz}$, $4_ym_zm_{zx}$, $4_z/m_z$, $2^{\star}_xm^{\star}_ym_z(2)$, $m^{\star}_{x\bar{y}}2^{\star}_{xy}m_z(2)$, $2^{\star}_z/m_z$	24	8	24	12
	m_{xy} $(m_{yz}, m_{zx}, m_{x\bar{y}}, m_{y\bar{z}}, m_{z\bar{x}})$	T_{1u}	$m_{x\bar{y}}m_{xy}m_z$	$m\bar{3}m$, $\bar{4}3m$, $\bar{4}_z2_xm_{xy}$, $4_zm_xm_{xy}$, $\bar{3}_rm_{xy}$, $\bar{3}_sm_{xy}$, 3_rm_{xy}, 3_sm_{xy}, $m^{\star}_{x\bar{y}}m_{xy}2^{\star}_z$, $2^{\star}_{xy}/m_{xy}$	24	4	24	12
	2_z $(2_x, 2_y)$	Reducible	$4_z/m_zm_xm_{x\bar{y}}$	$m\bar{3}$, 23, $\bar{4}_y2_zm_{zx}$, $4_y2_z2_{zx}$, $\bar{4}^{\star}_z$, $4^{\star}_z$, $m^{\star}_xm^{\star}_y2_z$, $m^{\star}_{x\bar{y}}m^{\star}_{xy}2_z$, $2^{\star}_x2^{\star}_y2_z$, $2^{\star}_{x\bar{y}}2^{\star}_{xy}2_z$, $2_z/m^{\star}_z$	24	8	6	12
	2_{xy} $(2_{yz}, 2_{zx}, 2_{x\bar{y}}, 2_{y\bar{z}}, 2_{z\bar{x}})$	T_{2u}	$m_{x\bar{y}}m_{xy}m_z$	$m\bar{3}m$, 432, $\bar{3}_rm_{xy}$, $\bar{3}_sm_{xy}$, 3_r2_{xy}, 3_s2_{xy}, $\bar{4}_zm_x2_{xy}$, $4_z2_x2_{xy}$, $m^{\star}_{x\bar{y}}2_{xy}m^{\star}_z$, $2^{\star}_{x\bar{y}}2_{xy}2^{\star}_z$, $2_{xy}/m^{\star}_{xy}$	24	4	12	12
	$\bar{1}$	T_{1g}, T_{2g}	$m\bar{3}m$	$\bar{3}_p(4)$, $4_z/m_z(3)$, $2^{\star}_z/m^{\star}_z(3)$, $2^{\star}_{xy}/m^{\star}_{xy}(6)$	24	24	0	24
	1	T_{1u}, T_{2u}	$m\bar{3}m$	$\bar{3}_p(4)$, $\bar{4}_z(3)$, $4_z(3)$, $m^{\star}_z(3)$, $m^{\star}_{xy}(6)$, $2^{\star}_z(3)$, $2^{\star}_{xy}(6)$, $\bar{1}^{\star}$	48	48	48	24

ferroic (low-symmetry) phase by $\mathcal{F}_1$, which is a proper subgroup of $\mathcal{G}$, $\mathcal{F}_1 \subset \mathcal{G}$. Further we denote by S_1 a *basic* (*microscopic*) low-symmetry structure described by positions of atoms in the unit cell. The stabilizer $\mathcal{I}_{\mathcal{G}}(\mathsf{S}_1)$ of the basic structure S_1 in a single-domain orientation is equal to the space group $\mathcal{F}_1$ of the ferroic (low-symmetry) phase,

$$\mathcal{I}_{\mathcal{G}}(\mathsf{S}_1) = \mathcal{F}_1. \qquad (3.4.2.41)$$

By applying a lost symmetry operation g_j on S_1, one gets a crystallographically equivalent low-symmetry basic structure S_j,

$$\mathsf{g}_j\mathsf{S}_1 = \mathsf{S}_j \neq \mathsf{S}_1, \quad \mathsf{g}_j \in \mathcal{G}, \quad \mathsf{g}_j \notin \mathcal{F}_1. \qquad (3.4.2.42)$$

We may recall that g_j is a space-group symmetry operation consisting of a rotation (point-group operation) g_j and a non-primitive translation $\mathbf{u}(g_j)$, $\mathsf{g}_j = \{g_j|\mathbf{u}(g_j)\}$ (see Section 1.2.3). The symbol $\{g_j|\mathbf{u}(g_j)\}$ is called a *Seitz space-group symbol* (Bradley & Cracknell, 1972). The product (composition law) of two Seitz symbols is

$$\{g_1|\mathbf{u}(g_1)\}\{g_2|\mathbf{u}(g_2)\} = \{g_1g_2|g_1\mathbf{u}(g_2) + \mathbf{u}(g_1)\}. \qquad (3.4.2.43)$$

All crystallographically equivalent low-symmetry basic structures form a $\mathcal{G}$-orbit and can be calculated from the first basic structure S_1 in the following way:

$$\mathcal{G}\mathsf{S}_1 = \{\mathsf{S}_1, \mathsf{S}_2, \ldots, \mathsf{S}_j \ldots, \mathsf{S}_N\} = \{\mathsf{e}\mathsf{S}_1, \mathsf{g}_2\mathsf{S}_1, \ldots, \mathsf{g}_j\mathsf{S}_1 \ldots, \mathsf{g}_N\mathsf{S}_1\}, \qquad (3.4.2.44)$$

where $\mathsf{g}_1 = \mathsf{e}$, $\mathsf{g}_2, \ldots, \mathsf{g}_j, \ldots, \mathsf{g}_N$ are the representatives of the left cosets $\mathsf{g}_j\mathcal{F}_1$ of the decomposition of $\mathcal{G}$,

$$\mathcal{G} = \mathcal{F}_1 \cup \mathsf{g}_2\mathcal{F}_1 \cup \ldots \cup \mathsf{g}_j\mathcal{F}_1 \cup \ldots \cup \mathsf{g}_N\mathcal{F}_1. \qquad (3.4.2.45)$$

These crystallographically equivalent low-symmetry structures are called *basic* (*elementary*) *domain states*.

The number N of basic domain states is equal to the number of left cosets in the decomposition (3.4.2.45). As we shall see in next section, this number is finite [see equation (3.4.2.60)], though the groups $\mathcal{G}$ and $\mathcal{F}_1$ consist of an infinite number of operations.

In a microscopic description, a *basic (elementary) domain state* is described by positions of atoms in the unit cell. Basic domain states that are related by translations suppressed at the phase transition are called *translational* or *antiphase domain states*. These domain states have the same macroscopic properties. The attribute 'to have the same macroscopic properties' divides all basic domain states into classes of translational domain states.

In a microscopic description, a ferroic phase transition is accompanied by a lowering of space-group symmetry from a parent space group $\mathcal{G}$, with translation subgroup $\mathcal{T}$ and point group G, to a low-symmetry space group $\mathcal{F}_1$, with translation subgroup $\mathcal{U}_1$ and point group F_1. There exists a unique intermediate group $\mathcal{M}_1$, called the *Hermann group*, which has translation subgroup $\mathcal{T}$ and point group $M_1 = F_1$ (see *e.g.* Hahn & Wondratschek, 1994; Wadhawan, 2000; Wondratschek & Aroyo, 2001):

$$\mathcal{F}_1 \overset{c}{\subseteq} \mathcal{M}_1 \overset{t}{\subseteq} \mathcal{G}, \qquad (3.4.2.46)$$

$$F_1 = M_1 \subseteq G, \qquad (3.4.2.47)$$

$$\mathcal{U}_1 \subseteq \mathcal{T} = \mathcal{T}, \qquad (3.4.2.48)$$

where $\overset{c}{\subset}$ denotes an equiclass subgroup (a descent at which only the translational subgroup is reduced but the point group is preserved) and $\overset{t}{\subset}$ signifies a equitranslational subgroup (only the point group descends but the translational subgroup does not change). Group $\mathcal{M}_1$ is a maximal subgroup of $\mathcal{G}$ that preserves all macroscopic properties of the basic domain state S_1 with symmetry $\mathcal{F}_1$.

At this point we have to make an important note. Any space-group symmetry descent $\mathcal{G} \subset \mathcal{F}_1$ requires that the lengths of the basis vectors of the translation group $\mathcal{U}_1$ of the ferroic space group $\mathcal{F}_1$ are commensurate with basic vectors of the translational group $\mathcal{T}$ of the parent space group $\mathcal{G}$. It is usually tacitly assumed that this condition is fulfilled, although in real phase transitions this is never the case. Lattice parameters depend on temperature and are, therefore, different in parent and ferroic phases. At ferroelastic phase transitions the spontaneous strain changes the lengths of the basis vectors in different ways and at first-order phase transitions the lattice parameters change abruptly.

To assure the validity of translational symmetry descents, we have to suppress all distortions of the crystal lattice. This condition, called the *high-symmetry approximation* (Zikmund, 1984) or *parent clamping approximation* (PCA) (Janovec *et al.*, 1989; Wadhawan, 2000), requires that the lengths of the basis vectors $\mathbf{a}^f\ \mathbf{b}^f\ \mathbf{c}^f$ of the translation group $\mathcal{U}_1$ of the ferroic space group $\mathcal{F}_1$ are either exactly the same as, or are integer multiples of, the basic vectors $\mathbf{a}^p\ \mathbf{b}^p\ \mathbf{c}^p$ of the translational group $\mathcal{T}$ of the parent space group $\mathcal{G}$. Then the relation between the primitive basis vectors $\mathbf{a}^f\ \mathbf{b}^f\ \mathbf{c}^f$ of $\mathcal{U}_1$ and the primitive basis vectors $\mathbf{a}^p\ \mathbf{b}^p\ \mathbf{c}^p$ of $\mathcal{T}$ can be expressed as

$$\left(\mathbf{a}^f,\ \mathbf{b}^f,\ \mathbf{c}^f\right) = \left(\mathbf{a}^p,\ \mathbf{b}^p,\ \mathbf{c}^p\right)\begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{13} & m_{23} & m_{33} \end{pmatrix}, \qquad (3.4.2.49)$$

where m_{ij}, $i, j = 1, 2, 3$, are integers.

Throughout this part, the parent clamping approximation is assumed to be fulfilled.

Now we can return to the partition of the set of basic domain states into translational subsets. Let $\{\mathsf{S}_1, \mathsf{S}_2, \ldots, \mathsf{S}_{d_t}\}$ be the set of all basic translational domain states that can be generated from S_1 by lost translations. The stabilizer (in $\mathcal{G}$) of this set is the Hermann group,

$$\mathcal{I}_{\mathcal{G}}\{\mathsf{S}_1, \mathsf{S}_2, \ldots, \mathsf{S}_{d_t}\} = \mathcal{M}_1, \qquad (3.4.2.50)$$

which plays the role of the intermediate group. The number of translational subsets and the relation between these subsets is determined by the decomposition of $\mathcal{G}$ into left cosets of $\mathcal{M}_1$:

$$\mathcal{G} = \{g_1|\mathbf{v}(g_1)\}\mathcal{M}_1 \cup \{g_2|\mathbf{v}(g_2)\}\mathcal{M}_1 \cup \ldots \cup \{g_j|\mathbf{v}(g_j)\}\mathcal{M}_1 \cup \ldots \cup \{g_n|\mathbf{v}(g_n)\}\mathcal{M}_1. \qquad (3.4.2.51)$$

Representatives $\mathsf{g}_j = \{g_j|\mathbf{u}(g_j)\}$ are space-group operations, where g_j is a point-group operation and $\mathbf{u}(g_j)$ is a non-primitive translation (see Section 1.2.3).

We note that the Hermann group $\mathcal{M}_1$ can be found in the software *GI★KoBo*-1 as the equitranslational subgroup of $\mathcal{G}$ with the point-group descent $G \subset F_1$ for any space group $\mathcal{G}$ and any point group F_1 of the ferroic phase.

The decomposition of the point group G into left cosets of the point group F_1 is given by equation (3.4.2.10):

$$G = g_1F_1 \cup g_2F_1 \cup \ldots \cup g_jF_1 \cup \ldots \cup g_nF_1. \qquad (3.4.2.52)$$

Since the space groups $\mathcal{M}_1$ and $\mathcal{F}_1$ have identical point groups, $M_1 = F_1$, the decomposition (3.4.2.51) is identical with a decomposition of G into left cosets of M_1; one can, therefore, choose for the representatives in (3.4.2.10) the point-group parts of the representatives $\{g_j|\mathbf{u}(g_j)\}$ in decomposition (3.4.2.51). Both decompositions comprise the same number of left cosets, *i.e.* corresponding indices are equal; therefore, the number of subsets, comprising only translational basic domain states, is equal to the number n of principal domain states:

$$n = [\mathcal{G} : \mathcal{M}_1] = [G : F_1] = |G| : |F_1|, \qquad (3.4.2.53)$$

where $|G|$ and $|F_1|$ are the number of operations of G and F_1, respectively.

The first 'representative' basic domain state S_j of each subset can be obtained from the first basic domain state S_1:

$$\mathsf{S}_j = \{g_j|\mathbf{v}(g_j)\}\mathsf{S}_1, \quad j = 1, 2, \ldots, n, \qquad (3.4.2.54)$$

where $\{g_j|\mathbf{v}(g_j)\}$ are representatives of left cosets of $\mathcal{M}_1$ in the decomposition (3.4.2.51).

Now we determine basic domain states belonging to the first subset (first principal domain state). Equiclass groups $\mathcal{M}_1$ and $\mathcal{F}_1$ have the same point-group operations and differ only in translations. The decomposition of $\mathcal{M}_1$ into left cosets of $\mathcal{F}_1$ can therefore be written in the form

$$\mathcal{M}_1 = \{e|\mathbf{t}_1\}\mathcal{F}_1 \cup \{e|\mathbf{t}_2\}\mathcal{F}_1 \cup \ldots \cup \{e|\mathbf{t}_k\}\mathcal{F}_1 \cup \ldots \cup \{e|\mathbf{t}_{d_t}\}\mathcal{F}_1, \qquad (3.4.2.55)$$

where e is the identity point-group operation and $\mathcal{T}_k$, $k = 1, 2 \ldots, d_t$, are lost translations that can be identified with the representatives in the decomposition of $\mathcal{T}$ into left cosets of $\mathcal{U}_1$:

$$\mathcal{T} = \mathbf{t}_1\mathcal{U}_1 + \mathbf{t}_2\mathcal{U}_1 + \ldots + \mathbf{t}_k\mathcal{U}_1 + \ldots + \mathbf{t}_{d_t}\mathcal{U}_1. \qquad (3.4.2.56)$$

The number d_t of basic domain states belonging to one principal domain state will be called a *translational degeneracy*. For the translations $\mathbf{t}_1, \mathbf{t}_2, \ldots, \mathbf{t}_k, \ldots, \mathbf{t}_{d_t}$, one can choose vectors that lead from the origin of a 'superlattice' primitive unit cell of $\mathcal{U}_1$ to lattice points of $\mathcal{T}$ located within or on the side faces of this 'superlattice' primitive unit cell. The number d_t of such lattice points is equal to the ratio $v_{\mathcal{F}} : v_{\mathcal{G}}$, where $v_{\mathcal{F}}$ and $v_{\mathcal{G}}$ are the volumes of the *primitive* unit cells of the low-symmetry and parent phases, respectively.

The number d_t can be also expressed as the determinant $\det(m_{ij})$ of the (3×3) matrix of the coefficients m_{ij} that in equation (3.4.2.49) relate the primitive basis vectors $\mathbf{a}^f, \mathbf{b}^f, \mathbf{c}^f$ of $\mathcal{U}_1$ to the primitive basis vectors $\mathbf{a}^p, \mathbf{b}^p, \mathbf{c}^p$ of $\mathcal{T}$ (Van Tendeloo & Amelinckx, 1974; see also Example 2.5 in Section 3.2.3.3). Finally, the number d_t equals the ratio $Z_{\mathcal{F}} : Z_{\mathcal{G}}$, where $Z_{\mathcal{F}}$ and $Z_{\mathcal{G}}$ are the numbers of chemical formula units in the *primitive* unit cell of the ferroic and parent phases, respectively. Thus we get for the translational degeneracy d_f three expressions:

$$d_t = [\mathcal{M}_1 : \mathcal{F}_1] = [\mathcal{T} : \mathcal{U}] = v_{\mathcal{F}} : v_{\mathcal{G}} = \det(m_{ij}) = Z_{\mathcal{F}} : Z_{\mathcal{G}}. \qquad (3.4.2.57)$$

The basic domain states belonging to the first subset of translational domain states are

$$\mathsf{S}_j = \{e|\mathbf{t}_k\}\mathsf{S}_1, \quad k = 1, 2, \ldots, d_t, \qquad (3.4.2.58)$$

where $\{e|\mathbf{t}_k\}$ is a representative from the decomposition (3.4.2.55).

The partitioning we have just described provides a useful labelling of basic domain states: Any basic domain state can be given a label ab, where the first integer $a = 1, 2, \ldots, n$ specifies the principal domain state (translational subset) and the integer $b = 1, 2, \ldots, d_t$ designates the the domain state within a subset. With this convention the kth basic domain state in the jth subset can be obtained from the first basic domain state $\mathsf{S}_1 = \mathsf{S}_{11}$ (see Proposition 3.2.3.30 in Section 3.2.3.3):

$$\mathsf{S}_{jk} = \{g_j|\mathbf{v}(g_j)\}\{e|\mathbf{t}_k\}\mathsf{S}_{11}, \quad j = 1, 2, \ldots, n, \quad k = 1, 2, \ldots, d_t. \qquad (3.4.2.59)$$

In a shorthand version, the letter S can be omitted and the symbol can be written in the form a_b, where the 'large' number a signifies the principal domain state and the subscript b (translational index) specifies a basic domain state compatible with the principal domain state a.

The number n of translational subsets (which can be associated with principal domain states) times the translational degeneracy d_t (number of translational domain states within one translational subset) is equal to the total number N of all basic domain states:

$$N = nd_t = (|G| : |F_1|)(v_{\mathcal{F}} : v_{\mathcal{G}}) = (|G| : |F_1|)\det(m_{ij}) = (|G| : |F_1|)(Z_{\mathcal{F}} : Z_{\mathcal{G}}). \qquad (3.4.2.60)$$

Example 3.4.2.6. Basic domain states in gadolinium molybdate (GMO). Gadolinium molybdate [$Gd_2(MoO_4)_3$] undergoes a non-equitranslational ferroic phase transition with parent space group $\mathcal{G} = P\bar{4}2_1m$ (D_{2d}^3) and with ferroic space group $\mathcal{F}_1 = Pba2$ (C_{2v}^8) (see Section 3.1.2). From equation (3.4.2.53) we get $n = |\bar{4}2m| : |mm2| = 8 : 4 = 2$, *i.e.* there are two subsets of translational domain states corresponding to two principal domain states. In the software *GI⋆KoBo*-1 one finds for the space group $P\bar{4}2_1m$ and the point group $mm2$ the corresponding equitranslational subgroup $\mathcal{M}_1 = Cmm2$ (C_{2v}^{11}) with vectors of the conventional orthorhombic unit cell (in the parent clamping approximation) $\mathbf{a}^o = \mathbf{a}^t - \mathbf{b}^t$, $\mathbf{b}^o = \mathbf{a}^t + \mathbf{b}^t$, $\mathbf{c}^o = \mathbf{c}^t$, where $\mathbf{a}^t, \mathbf{b}^t, \mathbf{c}^t$ is the basis of the tetragonal space group $P\bar{4}2_1m$. Hence, according to equation (3.4.2.49),

$$\begin{pmatrix} \mathbf{a}^o, & \mathbf{b}^o, & \mathbf{c}^o \end{pmatrix} = \begin{pmatrix} \mathbf{a}^t, & \mathbf{b}^t, & \mathbf{c}^t \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \qquad (3.4.2.61)$$

The determinant of the transformation matrix equals two, therefore, according to equation (3.4.2.57), each principal domain state can contain $d_t = 2$ translational domain states that are related by lost translation $\mathbf{a}^t$ or $\mathbf{b}^t$. In all, there are four basic domain states (for more details see Barkley & Jeitschko, 1973; Janovec, 1976; Wondratschek & Jeitschko, 1976).

Example 3.4.2.7. Basic domain states in calomel crystals. Crystals of calomel, Hg_2Cl_2, consist of almost linear Cl—Hg—Hg—Cl molecules aligned parallel to the c axis. The centres of gravity of these molecules form in the parent phase a tetragonal body-centred parent phase with the conventional tetragonal basis $\mathbf{a}^t, \mathbf{b}^t, \mathbf{c}^t$ and with space group $\mathcal{G} = I4/mmm$. The structure of this phase projected onto the $z = 0$ plane is depicted in the middle of Fig. 3.4.2.5 as a solid square with four full circles and one empty circle representing the centres of gravity of the Hg_2Cl_2 molecules at the levels $z = 0$ and $z = c/2$, respectively.

The ferroic phase has point-group symmetry $F_1 = m_{xy}m_{x\bar{y}}2_z$, hence there are $n = |\bar{4}2m| : |m_{xy}m_{x\bar{y}}2_z| = 2$ ferroelastic principal domain states. The conventional orthorhombic basis is $\mathbf{a}^o = \mathbf{a}^t - \mathbf{b}^t$, $\mathbf{b}^o = \mathbf{a}^t + \mathbf{b}^t$, $\mathbf{c}^o = \mathbf{c}^t$ (see upper left corner of Fig. 3.4.2.5). This is the same situation as in the previous example, therefore, according to equations (3.4.2.57) and (3.4.2.61), the translational degeneracy $d_t = 2$, *i.e.* each ferroelastic domain state can contain two basic domain states.

The structure S_1 of the ferroic phase in the parent clamping approximation is depicted in the left-hand part of Fig. 3.4.2.5 with a dotted orthorhombic conventional unit cell. The arrows represent exaggerated spontaneous shifts of the molecules. These shifts are frozen-in displacements of a transverse acoustic soft mode with the $\mathbf{k}$ vector along the [110] direction in the first domain state S_1, hence all molecules in the (110) plane passing through the origin O are shifted along the $[1\bar{1}0]$ direction, whereas those in the neighbouring parallel planes are shifted along the antiparallel direction $[\bar{1}10]$ (the indices are related to the tetragonal coordinate system). The symmetry of S_1 is described by the space group $\mathcal{F}_1 = Amam$ (D_{2h}^{17}); this symbol is related to the conventional orthorhombic basis and the origin of

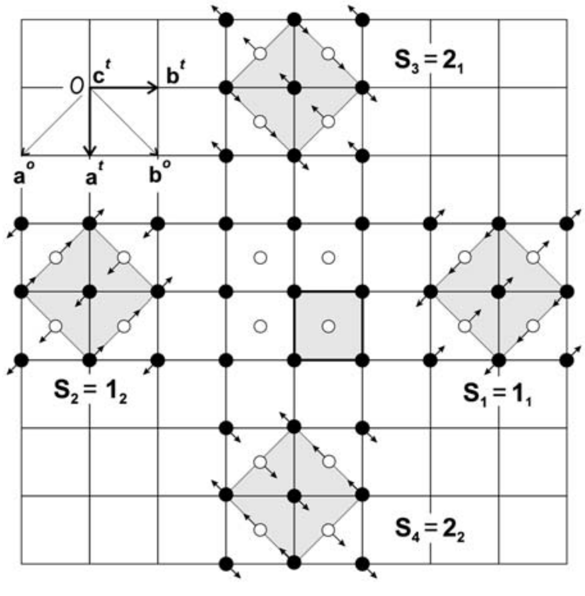

Fig. 3.4.2.5. Four basic single-domain states $S_1 = 1_1$, $S_2 = 1_2$, $S_3 = 2_1$, $S_4 = 2_2$ of the ferroic phase of a calomel (Hg_2Cl_2) crystal. Full • and empty ○ circles represent centres of gravity of Hg_2Cl_2 molecules at the levels $z = 0$ and $z = c/2$, respectively, projected onto the $z = 0$ plane. The parent tetragonal phase is depicted in the centre of the figure with a full square representing the primitive unit cell. Arrows are exaggerated spontaneous shifts of molecules in the ferroic phase. Dotted squares depict conventional unit cells of the orthorhombic basic domain states in the parent clamping approximation. If the parent clamping approximation is lifted, these unit cells would be represented by rectangles elongated parallel to the arrows.

this group is shifted by $\mathbf{a}^t/2$ or $\mathbf{b}$ with respect to the origin 0 of the group $\mathcal{G} = I4/mmm$.

Three more basic domain states S_2, S_3 and S_4 can be obtained, according to equation (3.4.2.44), from S_1 by applying representatives of the left cosets in the resolution of $\mathcal{G}$ [see equation (3.4.2.42)], for which one can find the expression

$$\mathcal{G} = \{1|000\}\mathcal{F}_1 \cup \{1|100\}\mathcal{F}_1 \cup \{4_z|000\}\mathcal{F}_1 \cup \{4_z{}^3|000\}\mathcal{F}_1. \quad (3.4.2.62)$$

All basic domain states S_1, S_2, S_3 and S_4 are depicted in Fig. 3.4.2.5. Domain states S_1 and S_2, and similarly S_3 and S_4, are related by lost translation $\mathbf{a}^t$ or $\mathbf{b}^t$. Thus the four basic domain states S_1, S_2, S_3 and S_4 can be partitioned into two translational subsets $\{S_1, S_2\}$ and $\{S_3, S_4\}$. Basic domain states forming one subset have the same value of the secondary macroscopic order parameter λ, which is in this case the difference $\varepsilon_{11} - \varepsilon_{22}$ of the components of a symmetric second-rank tensor ε, *e.g.* the permittivity or the spontaneous strain (which is zero in the parent clamping approximation).

This partition provides a useful labelling of basic domain states: $S_1 = 1_1$, $S_2 = 1_2$, $S_3 = 2_1$, $S_1 = 2_2$, where the first number signifies the ferroic (orientational) domain state and the subscript (translational index) specifies the basic domain state with the same ferroic domain state.

Symmetry groups (stabilizers in $\mathcal{G}$) of basic domain states can be calculated from a space-group version of equation (3.4.2.13):

$$\mathcal{F}_2 = \{1|100\}\mathcal{F}_2\{1|100\}^{-1} = \mathcal{F}_1;$$
$$\mathcal{F}_3 = \{4_z|000\}\mathcal{F}_2\{4_z|000\}^{-1} = Bbmm,$$

with the same conventional basis, and $\mathcal{F}_4 = \{1|100\}\mathcal{F}_3\{1|100\}^{-1} = \mathcal{F}_3$, where the origin of these groups is shifted by $\mathbf{a}^t/2$ or $\mathbf{b}$ with respect to the origin 0 of the group $\mathcal{G} = I4/mmm$.

In general, a space-group-symmetry descent $\mathcal{G} \supset \mathcal{F}_1$ can be performed in two steps:

(1) An equitranslational symmetry descent $\mathcal{G} \overset{t}{\supseteq} \mathcal{M}_1$, where $\mathcal{M}_1$ is the equitranslational subgroup of $\mathcal{G}$ (Hermann group), which is unequivocally specified by space group $\mathcal{G}$ and by the point group F_1 of the space group $\mathcal{F}_1$. The Hermann group $\mathcal{M}_1$ can be found in the software *GI★KoBo*-1 or, in some cases, in *IT* A (2005) under the entry 'Maximal non-isomorphic subgroups, type I'.

(2) An equiclass symmetry descent $\mathcal{M}_1 \overset{c}{\supseteq} \mathcal{F}_1$, which can be of three kinds [for more details see *IT* A (2005), Section 2.2.15]:

(i) Space groups $\mathcal{M}_1$ and $\mathcal{F}_1$ have the same conventional unit cell. These descents occur only in space groups $\mathcal{M}_1$ with centred conventional unit cells and the lost translations are some or all centring translations of the unit cell of $\mathcal{M}_1$. In many cases, the descent $\mathcal{M}_1 \overset{c}{\supseteq} \mathcal{F}_1$ can be found in the main tables of *IT* A (2005), under the entry 'Maximal non-isomorphic subgroups, type IIa'. Gadolinium molybdate belongs to this category.

(ii) The conventional unit cell of $\mathcal{M}_1$ is larger than that of $\mathcal{F}_1$. Some vectors of the conventional unit cell of $\mathcal{U}_1$ are multiples of that of $\mathcal{T}$. In many cases, the descent $\mathcal{M}_1 \overset{c}{\supseteq} \mathcal{F}_1$ can be found in the main tables of *IT* A (2005), under the entry 'Maximal non-isomorphic subgroups, type IIb'.

(iii) Space group $\mathcal{F}_1$ is an isomorphic subgroup of $\mathcal{M}_1$, *i.e.* both groups are of the same space-group type (with the same Hermann–Mauguin symbol) or of the enantiomorphic space-group type. Each space group has an infinite number of isomorphic subgroups. Maximal isomorphic subgroups of lowest index are tabulated in *IT* A (2005), under the entry 'Maximal non-isomorphic subgroups, type IIc'.

3.4.3. Domain pairs: domain twin laws, distinction of domain states and switching

Different domains observed by a single apparatus can exhibit different properties even though their crystal structures are either the same or enantiomorphic and differ only in spatial orientation. Domains are usually distinguished by their bulk properties, *i.e.* according to their domain states. Then the problem of domain distinction is reduced to the distinction of domain states. To solve this task, we have to describe in a convenient way the distinction of any two of all possible domain states. For this purpose, we use the concept of domain pair.

Domain pairs allow one to express the geometrical relationship between two domain states (the 'twin law'), determine the distinction of two domain states and define switching fields that may induce a change of one state into the other. Domain pairs also present the first step in examining domain twins and domain walls.

In this section, we define domain pairs, ascribe to them symmetry groups and so-called twinning groups, and give a classification of domain pairs. Then we divide domain pairs into equivalence classes (*G*-orbits of domain pairs) – which comprise domain pairs with the same inherent properties but with different orientations and/or locations in space – and examine the relation between *G*-orbits and twinning groups.

A qualitative difference between the coexistence of two domain states provides a basic division into non-ferroelastic and ferroelastic domain pairs. The synoptic Table 3.4.3.4 lists representatives of all *G*-orbits of *non-ferroelastic domain pairs*, contains information about the distinction of non-ferroelastic domain states by means of diffraction techniques and specifies whether or not important property tensors can distinguish between domain states of a non-ferroelastic domain pair. These data also determine the external fields needed to switch the first domain state into the second domain state of a domain pair. Synoptic Table 3.4.3.6 contains representative *ferroelastic domain pairs* of *G*-orbits of domain pairs for which there exist compatible (permissible) domain walls and gives for each representative pair the orientation of the *two compatible domain walls*, the expres-