

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

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_{ij} piezoelectric tensor; A_{ij} electrogyration tensor; $\pi_{\mu\nu}$ piezo-optic tensor ($i = 1, 2, 3; \mu, \nu = 1, 2, \dots, 6$). 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		Principal tensor parameters	Domain states			
		F_1	n_F		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		Principal tensor parameters	Domain states			
		F_1	n_F		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		Principal tensor parameters	Domain states			
		F_1	n_F		n_f	n_a	n_e	
Parent symmetry G: $2_x 2_y 2_z D_2$								
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: $m_x m_y 2_z C_{2vz}$								
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: $m_x m_y m_z D_{2h}$								
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^-	$2_x 2_y 2_z$	D_2	1	$\varepsilon; g_1, g_2, g_3; d_{14}, d_{25}, d_{36}$	2	1	0
B_{1u}	x_2^-	$m_x m_y 2_z$	C_{2vz}	1	P_3	2	1	2
B_{3u}	x_3^-	$2_x m_y m_z$	C_{2vx}	1	P_1	2	1	2
B_{2u}	x_4^-	$m_x 2_y m_z$	C_{2vy}	1	P_2	2	1	2

(d) Tetragonal parent groups

R-irep Γ_η	Standard variables	Ferroic symmetry		Principal tensor parameters	Domain states			
		F_1	n_F		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

3.1. STRUCTURAL PHASE TRANSITIONS

Table 3.1.3.1 (cont.)

R-irep Γ_η	Standard variables	Ferroic symmetry			Principal tensor parameters	Domain states		
		F_1	n_F			n_f	n_a	n_e
Parent symmetry G: $4_2 2_{xy} D_{4z}$								
A_2	x_2	4_z	C_{4z}	1	P_3	2	1	2
B_1	x_3	$2_x 2_y 2_z$	D_2	1	$\delta u_1 = -\delta u_2$	2	2	0
B_2	x_4	$2_{xy} 2_{xy} 2_z$	\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: $4_2 m_x m_{xy} C_{4vz}$								
A_2	x_2	4_z	C_{4z}	1	$\varepsilon; g_1 = g_2, g_3; d_{14} = -d_{25}$	2	1	1
B_1	x_3	$m_x m_y 2_z$	C_{2vz}	1	$\delta u_1 = -\delta u_2$	2	2	1
B_2	x_4	$m_{xy} m_{xy} 2_z$	\hat{C}_{2vz}	1	u_6	2	2	1
E	$(x_1, 0)$	m_x	C_{xx}	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: $\bar{4}_2 2_x m_{xy} D_{2dz}$								
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	$2_x 2_y 2_z$	D_2	1	$\varepsilon; \delta u_1 = -\delta u_2$	2	2	0
B_2	x_4	$m_{xy} m_{xy} 2_z$	\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: $\bar{4}_2 m_x 2_{xy} \hat{D}_{2dz}$								
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	$m_x m_y 2_z$	C_{2vz}	1	$P_3; \delta u_1 = -\delta u_2$	2	2	2
B_1	x_4	$2_{xy} 2_{xy} 2_z$	\hat{D}_{2z}	1	$\varepsilon; u_6$	2	2	0
E	$(x_1, 0)$	m_x	C_{xx}	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: $4_z/m_x m_x m_{xy} D_{4hz}$								
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^+	$m_x m_y m_z$	\hat{D}_{2hz}	1	$\delta u_1 = -\delta u_2$	2	2	0
B_{2g}	x_4^+	$m_{xy} m_{xy} m_z$	\hat{D}_{2hz}	1	u_6	2	2	0
A_{1u}	x_1^-	$4_2 2_x 2_{xy}$	D_{4z}	1	$\varepsilon; g_1 = g_2, g_3; d_{14} = -d_{25}$	2	1	0
A_{2u}	x_2^-	$4_z m_x m_{xy}$	C_{4vz}	1	P_3	2	1	2
B_{1u}	x_3^-	$\bar{4}_z 2_x m_{xy}$	D_{2dz}	1	$g_1 = -g_2; d_{14} = d_{25}, d_{36}$	2	1	0
B_{2u}	x_4^-	$\bar{4}_z m_x 2_{xy}$	\hat{D}_{2dz}	1	$g_6; d_{31} = -d_{32}, d_{15} = -d_{24}$	2	1	0
E_g	$(x_1^+, 0)$	$2_x/m_x$	C_{2hx}	2	u_4	4	4	0
	(x_1^+, x_1^+)	$2_{xy}/m_{xy}$	C_{2hxy}	2	$u_4 = -u_5$	4	4	0
	(x_1^+, y_1^+)	1	C_i	1	$(u_4, -u_5)$	8	8	0
E_u	$(x_1^-, 0)$	$2_x m_y m_z$	C_{2vx}	2	P_1	4	2	4
	(x_1^-, x_1^-)	$m_{xy} 2_{xy} m_z$	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			Principal tensor parameters	Domain states		
		F_1	n_F			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
(La, Li)					$(u_1 - u_2, -2u_6), (u_4, -u_5)$ $\delta u_1 = -\delta u_2$			
Parent symmetry G: $\bar{3}_z C_{3i}$								
A_u	x_1^-	3_z	C_3	1	$\varepsilon; P_3$	2	1	2
E_g	(x_1^+, y_1^+)	$\bar{1}$	C_i	1	$(u_1 - u_2, -2u_6), (u_4, -u_5)$ $\delta u_1 = -\delta u_2$	3	3	0
(La)								
E_u	(x_1^-, y_1^-)	1	C_1	1	(P_1, P_2)	6	3	6
Parent symmetry G: $3_2 2_x D_{3x}$								
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: $3_2 m_x C_{3vx}$								
A_2	x_2	3_z	C_3	1	$\varepsilon; g_1 = g_2, g_3; d_{11} = -d_{12} = -d_{26}, d_{14} = -d_{25}$	2	1	1
E	$(x_1, 0)$	m_x	C_{3x}	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

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Table 3.1.3.1 (cont.)

R-irep Γ_η	Standard variables	Ferroic symmetry			Principal tensor parameters	Domain states		
		F_1	n_F			n_f	n_a	n_e
Parent symmetry G: $\bar{3}_2m_x D_{3dx}$								
A_{2g}	x_2^+	$\bar{3}_z$	C_{3i}	1	$A_{22} = -A_{21} = -A_{16}, A_{31} = A_{32}, A_{33}, A_{15} = A_{24}$ $\varepsilon; g_1 = g_2, g_3; d_{11} = -d_{12} = -d_{26}, d_{14} = -d_{25}$ P_3	2	1	0
A_{1u}	x_1^-	$3_z 2_x$	D_{3x}	1		2	1	0
A_{2u}	x_2^-	$3_z m_x$	C_{3vx}	1		2	1	2
E_g (La)	$(x_1^+, 0)$ (x_1^+, y_1^+)	$2_x/m_x$ $\bar{1}$	C_{2hx} C_i	3 1	$\delta u_1 = -\delta u_2, u_4$ $(u_1 - u_2, -2u_6), (u_4, -u_5)$	3 6	3 6	0 0
E_u	$(0, y_1^-)$ $(x_1^-, 0)$ (x_1^-, y_1^-)	m_x 2_x 1	C_{xx} C_{2x} C_1	3 3 1	P_2 P_1 (P_1, P_2)	6 6 12	3 3 6	6 6 12
Parent symmetry G: $3_2y D_{3y}$								
A_2	x_2	3_z	C_3	1	P_3	2	1	2
E (La, Li)	$(0, y_1)$ (x_1, y_1)	2_y 1	C_{2y} C_1	3 1	$P_2; \delta u_1 = -\delta u_2, u_5$ $(P_1, P_2); (2u_6, u_1 - u_2), (u_4, -u_5)$	3 6	3 6	3 6
Parent symmetry G: $3_2m_y C_{3vy}$								
A_2	x_2	3_z	C_3	1	$\varepsilon; g_1 = g_2, g_3; d_{22} = -d_{21} = -d_{16}, d_{14} = -d_{25}$	2	1	1
E (La)	$(0, y_1)$ (x_1, y_1)	m_y 1	C_{sy} C_1	3 1	$P_1; \delta u_1 = -\delta u_2, u_5$ $(P_2, -P_1); (2u_6, u_1 - u_2), (u_4, -u_5)$	3 6	3 6	3 6
Parent symmetry G: $\bar{3}_2m_y D_{3dy}$								
A_{2g}	x_2^+	$\bar{3}_z$	C_{3i}	1	$A_{11} = -A_{12} = -A_{26}, A_{31} = A_{32}, A_{33}, A_{15} = A_{24}$ $\varepsilon; g_1 = g_2, g_3; d_{22} = -d_{21} = -d_{16}, d_{14} = -d_{25}$ P_3	2	1	0
A_{1u}	x_1^-	$3_z 2_y$	D_{3y}	1		2	1	0
A_{2u}	x_2^-	$3_z m_y$	C_{3vy}	1		2	1	2
E_g (La)	$(0, y_1^+)$ (x_1^+, y_1^+)	$2_y/m_y$ $\bar{1}$	C_{2hy} C_i	3 1	$\delta u_1 = -\delta u_2, u_5$ $(2u_6, u_1 - u_2), (u_4, -u_5)$	3 6	3 6	0 0
E_u	$(0, y_1^-)$ $(x_1^-, 0)$ (x_1^-, y_1^-)	2_y m_y 1	C_{2y} C_{sy} C_1	3 3 1	P_2 P_1 (P_1, P_2)	6 6 12	3 3 6	6 6 12

(f) Hexagonal parent groups

Covariants with standardized labels and conversion equations:

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

R-irep Γ_η	Standard variables	Ferroic symmetry			Principal tensor parameters	Domain states		
		F_1	n_F			n_f	n_a	n_e
Parent symmetry G: $6_2 C_6$								
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: $\bar{6}_2 C_{3h}$								
A''	x_3	3_z	C_3	1	$\varepsilon; P_3$	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: $6_2/m_z C_{6h}$								
B_g	x_3^+	$\bar{3}_z$	C_{3i}	1	$A_{11} = -A_{12} = -A_{26}, A_{22} = -A_{21} = -A_{16}$ $\varepsilon; P_3$ $d_{11} = -d_{12} = -d_{26}, d_{22} = -d_{21} = -d_{16}$	2	1	0
A_u	x_1^-	6_z	C_6	1		2	1	2
B_u	x_3^-	$\bar{6}_z$	C_{3h}	1		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

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Table 3.1.3.1 (cont.)

R-irep Γ_η	Standard variables	Ferroic symmetry			Principal tensor parameters	Domain states		
		F_1	n_F			n_f	n_a	n_e
Parent symmetry G: $6_2 2_x 2_y D_6$								
A_2	x_2	6_z	C_6	1	P_3	2	1	2
B_1	x_3	$3_z 2_x$	D_{3x}	1	$d_{11} = -d_{12} = -d_{26}$	2	1	0
B_2	x_4	$3_z 2_y$	D_{3y}	1	$d_{22} = -d_{21} = -d_{16}$	2	1	0
E_2	$(x_2, 0)$	$2_x 2_y 2_z$	D_2	3	$\delta u_1 = -\delta u_2$	3	3	0
(La, Li)	(x_2, y_2)	2_z	C_{2z}	1	$(u_1 - u_2, 2u_6)$	6	6	2
E_1	$(x_1, 0)$	2_x	C_{2x}	3	$P_1; u_4$	6	6	6
	$(0, y_1)$	2_y	C_{2y}	3	$P_2; u_5$	6	6	6
(Li)	(x_1, y_1)	1	C_1	1	$(P_1, P_2); (u_4, -u_5)$	12	12	12
Parent symmetry G: $6_2 m_x m_y C_{6v}$								
A_2	x_2	6_z	C_6	1	$\varepsilon; g_1 = g_2, g_3; d_{14} = -d_{25}$	2	1	1
B_2	x_3	$3_z m_x$	C_{3vx}	1	$d_{22} = -d_{21} = -d_{16}$	2	1	1
B_1	x_4	$3_z m_y$	C_{3vy}	1	$d_{11} = -d_{12} = -d_{26}$	2	1	1
E_2	$(x_2, 0)$	$m_x m_y 2_z$	C_{2vz}	3	$\delta u_1 = -\delta u_2$	3	3	1
(La)	(x_2, y_2)	2_z	C_{2z}	1	$(u_1 - u_2, 2u_6)$	6	6	1
E_1	$(x_1, 0)$	m_x	C_{sx}	3	$P_2; u_4$	6	6	6
	$(0, y_1)$	m_y	C_{sy}	3	$P_1; u_5$	6	6	6
	(x_1, y_1)	1	C_1	1	$(P_2, -P_1); (u_4, -u_5)$	12	12	12
Parent symmetry G: $\bar{6}_2 2_x m_y D_{3h}$								
A'_2	x_2	$\bar{6}_z$	C_{3h}	1	$d_{22} = -d_{21} = -d_{16}$	2	1	0
A''_1	x_3	$3_z 2_x$	D_{3x}	1	$\varepsilon; g_1 = g_2, g_3; d_{14} = -d_{25}$	2	1	0
A''_2	x_4	$3_z m_y$	C_{3vy}	1	P_3	2	1	2
E'	$(x_2, 0)$	$2_x m_y m_z$	C_{2vx}	3	$P_1; \delta u_1 = -\delta u_2$	3	3	3
(La)	(x_2, y_2)	m_z	C_{sz}	1	$(P_1, -P_2); (u_1 - u_2, 2u_6)$	6	6	6
E''	$(x_1, 0)$	2_x	C_{2x}	3	u_4	6	6	3
	$(0, y_1)$	m_y	C_{sy}	3	u_5	6	6	6
	(x_1, y_1)	1	C_1	1	$(u_4, -u_5)$	12	12	12
Parent symmetry G: $\bar{6}_2 m_x 2_y \bar{D}_{3h}$								
A'_2	x_2	$\bar{6}_z$	C_{3h}	1	$d_{11} = -d_{12} = -d_{26}$	2	1	0
A''_2	x_3	$3_z m_x$	C_{3vx}	1	P_3	2	1	2
A'_1	x_4	$3_z 2_y$	D_{3y}	1	$\varepsilon; g_1 = g_2, g_3; d_{14} = -d_{25}$	2	1	0
E'	$(x_2, 0)$	$m_x 2_y m_z$	C_{2vy}	3	$P_2; \delta u_1 = -\delta u_2$	3	3	3
(La)	(x_2, y_2)	m_z	C_{sz}	1	$(P_2, P_1); (u_1 - u_2, 2u_6)$	6	6	6
E''	$(x_1, 0)$	m_x	C_{sx}	3	u_4	6	6	6
	$(0, y_1)$	2_y	C_{2y}	3	u_5	6	6	3
	(x_1, y_1)	1	C_1	1	$(u_4, -u_5)$	12	12	12
Parent symmetry G: $6_z/m_x m_y D_{6h}$								
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^+	$3_z m_x$	D_{3dx}	1	$A_{11} = -A_{12} = -A_{26}$	2	1	0
B_{2g}	x_4^+	$3_z m_y$	D_{3dy}	1	$A_{22} = -A_{21} = -A_{16}$	2	1	0
A_{1u}	x_1^-	$6_2 2_x 2_y$	D_6	1	$\varepsilon; g_1 = g_2, g_3; d_{14} = -d_{25}$	2	1	0
A_{2u}	x_2^-	$6_z m_x m_y$	C_{6v}	1	P_3	2	1	2
B_{1u}	x_3^-	$6_z 2_x m_y$	D_{3h}	1	$d_{11} = -d_{12} = -d_{26}$	2	1	0
B_{2u}	x_4^-	$6_z m_x 2_y$	\bar{D}_{3h}	1	$d_{22} = -d_{21} = -d_{16}$	2	1	0
E_{2g}	$(x_2^+, 0)$	$m_x m_y m_z$	D_{2h}	3	$\delta u_1 = -\delta u_2$	3	3	0
(La)	(x_2^+, y_2^+)	$2_z/m_z$	C_{2hz}	1	$(u_1 - u_2, 2u_6)$	6	6	0
E_{1g}	$(x_1^+, 0)$	$2_x/m_x$	C_{2hx}	3	u_4	6	6	0
	$(0, y_1^+)$	$2_y/m_y$	C_{2hy}	3	u_5	6	6	0
	(x_1^+, y_1^+)	1	C_i	1	$(u_4, -u_5)$	12	12	0
E_{1u}	$(x_1^-, 0)$	$2_x m_y m_z$	C_{2vx}	3	P_1	6	3	6
	$(0, y_1^-)$	$m_x 2_y m_z$	C_{2vy}	3	P_2	6	3	6
	(x_1^-, y_1^-)	m_z	C_{sz}	1	(P_1, P_2)	12	6	12
E_{2u}	$(x_2^-, 0)$	$2_x 2_y 2_z$	D_2	3	$\delta g_1 = -\delta g_2; d_{36}, \delta d_{14} = \delta d_{25}$	6	3	0
	$(0, y_2^-)$	$m_x m_y 2_z$	C_{2vz}	3	$g_6; d_{32} = -d_{31}, d_{24} = -d_{15}$	6	3	2
	(x_2^-, y_2^-)	2_z	C_{2z}	1	$(g_1 - g_2, 2g_6); (2d_{36}, d_{32} - d_{31}), (d_{14} + d_{25}, d_{24} - d_{15})$	12	6	2

In tensor distinction of domains, the secondary tensor parameters play a secondary role in a sense that some but not all ferroic domain states exhibit different values of the secondary tensor parameters. This property forms a basis for the concept of partial ferroic phases (Aizu, 1970): A ferroic phase is a *partial ferroelectric (ferroelastic)* one if some but not all domain states differ in spontaneous polarization (spontaneous strain). A non-ferroelectric phase denotes a ferroic phase which is either non-polar or which possesses a unique polar direction available

already in the parent phase. A non-ferroelastic phase exhibits no spontaneous strain.

3.1.3.3. Tables of equitranslational phase transitions associated with irreducible representations

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

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

Table 3.1.3.1 (cont.)

(g) Cubic parent groups

Covariants with standardized labels and conversion equations:

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

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

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

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

(1) *Inverse Landau problem* (Ascher & Kobayashi, 1977) of equitranslational phase transitions: For a given equitranslational symmetry descent $\mathcal{G} \Downarrow^t \mathcal{F}$ (determined for example from diffraction experiments), find the representation Γ_η of \mathcal{G} that specifies the transformation properties of the primary order parameter. Solution: In Table 3.1.3.1, one finds a physically irre-

ducible representation Γ_η of the point group G of \mathcal{G} with epikernel F (point group of \mathcal{F}). For some symmetry descents from cubic point groups $G = 432, 43m$ and $m\bar{3}m$, the inverse Landau problem has two solutions, which are given in Table 3.1.3.2.

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

3.1. STRUCTURAL PHASE TRANSITIONS

Table 3.1.3.1 (cont.)

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