International Tables for Crystallography (2006). Vol. D, Section 1.1.4.10, pp. 24–31.

(ii) Groups $m\bar{3}m$, 432, $\bar{4}3m$, and spherical system: the reduced tensors are already symmetric (see Sections 1.1.4.9.7 and 1.1.4.9.8).

1.1.4.10. *Reduced form of polar and axial tensors – matrix representation*

1.1.4.10.1. *Introduction*

Many tensors representing physical properties or physical quantities appear in relations involving symmetric tensors. Consider, for instance, the strain S_{ij} resulting from the application of an electric field **E** (the piezoelectric effect):

$$S_{ij} = d_{ijk}E_k + Q_{ijkl}E_kE_l, \qquad (1.1.4.4)$$

where the first-order terms d_{ijk} represent the components of the third-rank converse piezoelectric tensor and the second-order terms Q_{ijkl} represent the components of the fourth-rank electrostriction tensor. In a similar way, the direct piezoelectric effect corresponds to the appearance of an electric polarization **P** when a stress T_{jk} is applied to a crystal:

$$P_i = d_{ijk}T_{jk}. \qquad (1.1.4.5)$$

Owing to the symmetry properties of the strain and stress tensors (see Sections 1.3.1 and 1.3.2) and of the tensor product E_kE_l, there occurs a further reduction of the number of independent components of the tensors which are engaged in a contracted product with them, as is shown in Section 1.1.4.10.3 for third-rank tensors and in Section 1.1.4.10.5 for fourth-rank tensors.

1.1.4.10.2. *Stress and strain tensors – Voigt matrices*

The stress and strain tensors are symmetric because body torques and rotations are not taken into account, respectively (see Sections 1.3.1 and 1.3.2). Their components are usually represented using Voigt's one-index notation.

(i) Strain tensor

$$\left.\begin{array}{lll} S_1 = S_{11}; & S_2 = S_{22}; & S_3 = S_{33}; \\ S_4 = S_{23} + S_{32}; & S_5 = S_{31} + S_{13}; & S_6 = S_{12} + S_{21}; \\ S_4 = 2S_{23} = 2S_{32}; & S_5 = 2S_{31} = 2S_{13}; & S_6 = 2S_{12} = 2S_{21}. \end{array}\right\} \qquad (1.1.4.6)$$

The Voigt components S_α form a Voigt matrix:

$$\begin{pmatrix} S_1 & S_6 & S_5 \\ & S_2 & S_4 \\ & & S_3 \end{pmatrix}.$$

The terms of the leading diagonal represent the elongations (see Section 1.3.1). It is important to note that the non-diagonal terms, which represent the shears, are here equal to *twice* the corresponding components of the strain tensor. The components S_α of the Voigt strain matrix are therefore *not* the components of a tensor.

(ii) Stress tensor

$$\left.\begin{array}{lll} T_1 = T_{11}; & T_2 = T_{22}; & T_3 = T_{33}; \\ T_4 = T_{23} = T_{32}; & T_5 = T_{31} = T_{13}; & T_6 = T_{12} = T_{21}. \end{array}\right\}$$

The Voigt components T_α form a Voigt matrix:

$$\begin{pmatrix} T_1 & T_6 & T_5 \\ & T_2 & T_4 \\ & & T_3 \end{pmatrix}.$$

The terms of the leading diagonal correspond to principal normal constraints and the non-diagonal terms to shears (see Section 1.3.2).

1.1.4.10.3. *Reduction of the number of independent components of third-rank polar tensors due to the symmetry of the strain and stress tensors*

Equation (1.1.4.5) can be written

$$P_i = \sum_j d_{ijj}T_{jj} + \sum_{j\neq k}(d_{ijk} + d_{ikj})T_{jk}.$$

The sums $(d_{ijk} + d_{ikj})$ for $j \neq k$ have a definite physical meaning, but it is impossible to devise an experiment that permits d_{ijk} and d_{ikj} to be measured separately. It is therefore usual to set them equal:

$$d_{ijk} = d_{ikj}. \qquad (1.1.4.7)$$

It was seen in Section 1.1.4.8.1 that the components of a third-rank tensor can be represented as a 9×3 matrix which can be subdivided into three 3×3 submatrices:

$$(\ \mathbf{1}\ |\ \mathbf{2}\ |\ \mathbf{3}\ ).$$

Relation (1.1.4.7) shows that submatrices **1** and **2** are identical. One puts, introducing a two-index notation,

$$\left.\begin{array}{rl} d_{ijj} = d_{i\alpha} & (\alpha = 1, 2, 3) \\ d_{ijk} + d_{ikj}\ (j \neq k) = d_{i\alpha} & (\alpha = 4, 5, 6). \end{array}\right\}$$

Relation (1.1.4.7) becomes

$$P_i = d_{i\alpha}T_\alpha.$$

The coefficients $d_{i\alpha}$ may be written as a 3×6 matrix:

$$\left(\begin{array}{ccc|ccc} 11 & 12 & 13 & 14 & 15 & 16 \\ 21 & 22 & 23 & 24 & 25 & 26 \\ 31 & 32 & 33 & 34 & 35 & 36 \end{array}\right).$$

This matrix is constituted by two 3×3 submatrices. The left-hand one is identical to the submatrix **1**, and the right-hand one is equal to the sum of the two submatrices **2** and **3**:

$$(\ \mathbf{1}\ |\ \mathbf{2+3}\ ).$$

The inverse piezoelectric effect expresses the strain in a crystal submitted to an applied electric field:

$$S_{ij} = d_{ijk}E_k,$$

where the matrix associated with the coefficients d_{ijk} is a 9×3 matrix which is the transpose of that of the coefficients used in equation (1.1.4.5), as shown in Section 1.1.1.4.

The components of the Voigt strain matrix S_α are then given by

$$\left.\begin{array}{ll} S_\alpha = d_{iik}E_k & (\alpha = 1, 2, 3) \\ S_\alpha = S_{ij} + S_{ji} = (d_{ijk} + d_{jik})E_k & (\alpha = 4, 5, 6). \end{array}\right\}$$

This relation can be written simply as

$$S_\alpha = d_{\alpha k}E_k,$$

where the matrix of the coefficients $d_{\alpha k}$ is a 6×3 matrix which is the transpose of the $d_{i\alpha}$ matrix.

There is another set of piezoelectric constants (see Section 1.1.5) which relates the stress, T_{ij}, and the electric field, E_k, which are both intensive parameters:

$$T_{ij} = e_{ijk}E_k, \qquad (1.1.4.8)$$

where a new piezoelectric tensor is introduced, e_{ijk}. Its components can be represented as a 3×9 matrix:

$$\begin{pmatrix} \mathbf{1} \\ \hline \mathbf{2} \\ \hline \mathbf{3} \end{pmatrix}.$$

Both sides of relation (1.1.4.8) remain unchanged if the indices i and j are interchanged, on account of the symmetry of the stress tensor. This shows that

$$e_{ijk} = e_{jik}.$$

Submatrices **2** and **3** are equal. One introduces here a two-index notation through the relation $e_{\alpha k} = e_{ijk}$, and the $e_{\alpha k}$ matrix can be written

$$\left(\frac{\mathbf{1}}{\mathbf{2}+\mathbf{3}}\right).$$

The relation between the full and the reduced matrix is therefore different for the d_{ijk} and the e_{kij} tensors. This is due to the particular property of the strain Voigt matrix (1.1.4.6), and as a consequence the relations between nonzero components of the reduced matrices are different for certain point groups (3, 32, 3m, $\bar{6}$, $\bar{6}2m$).

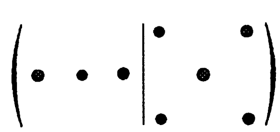
1.1.4.10.4. *Independent components of the matrix associated with a third-rank polar tensor according to the following point groups*

1.1.4.10.4.1. *Triclinic system*

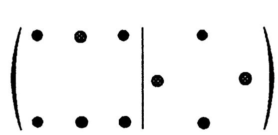
(i) Group 1: all the components are independent. There are 18 components.
(ii) Group $\bar{1}$: all the components are equal to zero.

1.1.4.10.4.2. *Monoclinic system*

(i) Group 2: twofold axis parallel to Ox_2:



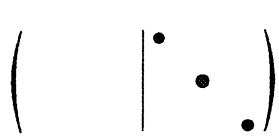
There are 8 independent components.
(ii) Group m:



There are 10 independent components.
(iii) Group $2/m$: all the components are equal to zero.

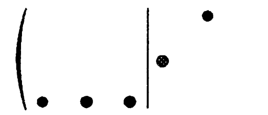
1.1.4.10.4.3. *Orthorhombic system*

(i) Group 222:



There are 3 independent components.

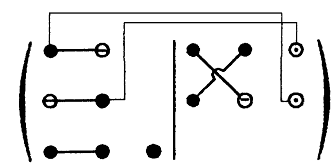
(ii) Group $mm2$:



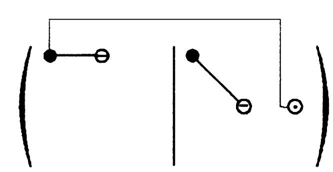
There are 5 independent components.
(iii) Group mmm: all the components are equal to zero.

1.1.4.10.4.4. *Trigonal system*

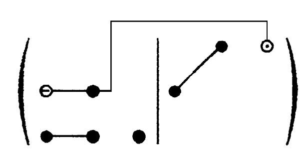
(i) Group 3:



where the symbol ⊖ means that the corresponding component is equal to the opposite of that to which it is linked, ⊙ means that the component is equal to twice minus the value of the component to which it is linked for d_{ijk} and to minus the value of the component to which it is linked for e_{ijk}. There are 6 independent components.
(ii) Group 32, twofold axis parallel to Ox_1:



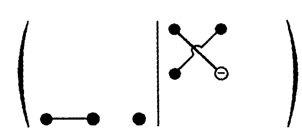
with the same conventions. There are 4 independent components.
(iii) Group 3m, mirror perpendicular to Ox_1:



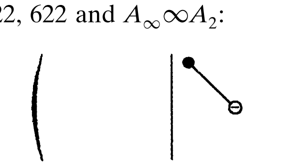
with the same conventions. There are 4 independent components.
(iv) Groups $\bar{3}$ and $\bar{3}m$: all the components are equal to zero.

1.1.4.10.4.5. *Tetragonal, hexagonal and cylindrical systems*

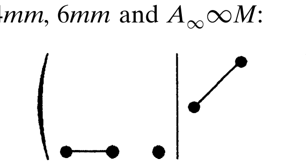
(i) Groups 4, 6 and A_∞:



There are 4 independent components.
(ii) Groups 422, 622 and $A_\infty \infty A_2$:



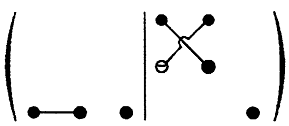
There is 1 independent component.
(iii) Groups 4mm, 6mm and $A_\infty \infty M$:



There are 3 independent components.

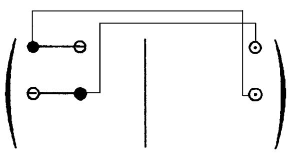
(iv) Groups $4/m$, $6/m$ and $(A_\infty/M)C$: all the components are equal to zero.

(v) Group $\bar{4}$:



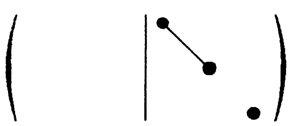
There are 4 independent components.

(vi) Group $\bar{6} = 3/m$:



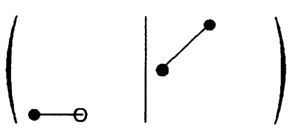
with the same conventions as for group 3. There are 2 independent components.

(vii) Group $\bar{4}2m$ – twofold axis parallel to Ox_1:



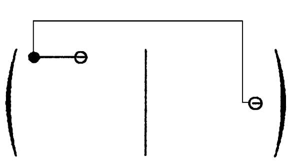
There are 2 independent components.

(viii) Group $\bar{4}2m$ – mirror perpendicular to Ox_1 (twofold axis at 45°):



The number of independent components is of course the same.

(ix) Group $\bar{6}2/m$:

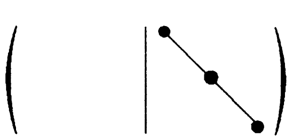


with the same conventions as for group 3. There is 1 independent component.

(x) Groups $4/mm$, $6/mm$ and $(A_\infty/M)\infty(A_2/M)C$: all the components are equal to zero.

1.1.4.10.4.6. *Cubic and spherical systems*

(i) Groups 23 and $\bar{4}3m$:



There is 1 independent component.

(ii) Groups 432 and ∞A_∞: it was seen in Section 1.1.4.8.6 that we have in this case

$$d_{123} = -d_{132}.$$

It follows that $d_{14} = 0$, all the components are equal to zero.

(iii) Groups $m3$, $m\bar{3}m$ and $\infty(A_\infty/M)C$: all the components are equal to zero.

1.1.4.10.5. *Reduction of the number of independent components of fourth-rank polar tensors due to the symmetry of the strain and stress tensors*

Let us consider five examples of fourth-rank tensors:

(i) *Elastic compliances*, s_{ijkl}, relating the resulting strain tensor S_{ij} to an applied stress T_{ij} (see Section 1.3.3.2):

$$S_{ij} = s_{ijkl} T_{kl}, \qquad (1.1.4.9)$$

where the compliances s_{ijkl} are the components of a tensor of rank 4.

(ii) *Elastic stiffnesses*, c_{ijkl} (see Section 1.3.3.2):

$$T_{ij} = c_{ijkl} S_{kl}.$$

(iii) *Piezo-optic coefficients*, π_{ijkl}, relating the variation $\Delta\eta_{ij}$ of the dielectric impermeability to an applied stress T_{kl} (*photoelastic effect* – see Section 1.6.7):

$$\Delta\eta_{ij} = \pi_{ijkl} T_{kl}.$$

(iv) *Elasto-optic coefficients*, p_{ijkl}, relating the variation $\Delta\eta_{ij}$ of the dielectric impermeability to the strain S_{kl}:

$$\Delta\eta_{ij} = p_{ijkl} S_{kl}.$$

(v) *Electrostriction coefficients*, Q_{ijkl}, which appear in equation (1.1.4.4):

$$S_{ij} = Q_{ijkl} E_k E_l, \qquad (1.1.4.10)$$

where only the second-order terms are considered.

In each of the equations from (1.1.4.9) to (1.1.4.10), the contracted product of a fourth-rank tensor by a symmetric second-rank tensor is equal to a symmetric second-rank tensor. As in the case of the third-rank tensors, this results in a reduction of the number of independent components, but because of the properties of the strain Voigt matrix, and because two of the tensors are endowed with intrinsic symmetry (the elastic tensors), the reduction is different for each of the five tensors. The above relations can be written in matrix form:

$$\left(\begin{array}{c} \mathbf{1} \\ \hline \mathbf{2} \\ \hline \mathbf{3} \end{array}\right) = \left(\begin{array}{c|c|c} \mathbf{1} & \mathbf{2} & \mathbf{3} \\ \hline \mathbf{4} & \mathbf{5} & \mathbf{6} \\ \hline \mathbf{7} & \mathbf{8} & \mathbf{9} \end{array}\right) \times \left(\begin{array}{c} \mathbf{1} \\ \hline \mathbf{2} \\ \hline \mathbf{3} \end{array}\right)$$

where the second-rank tensors are represented by 1×9 column matrices, which can each be subdivided into three 1×3 submatrices and the 9×9 matrix associated with the fourth-rank tensors is subdivided into nine 3×3 submatrices, as shown in Section 1.1.4.9.1. The symmetry of the second-rank tensors means that submatrices **2** and **3** which are associated with them are equal.

Let us first consider the reduction of the tensor of elastic compliances. As in the case of the piezoelectric tensor, equation (1.1.4.9) can be written

$$S_{ij} = \sum_l s_{ijll} T_{ll} + \sum_{k \neq l} (s_{ijkl} + s_{ijlk}) T_{kl}. \qquad (1.1.4.11)$$

The sums $(s_{ijkl} + s_{ijlk})$ for $k \neq l$ have a definite physical meaning, but it is impossible to devise an experiment permitting s_{ijkl} and s_{ijlk} to be measured separately. It is therefore usual to set them equal in order to avoid an unnecessary constant:

$$s_{ijkl} = s_{ijlk}.$$

Furthermore, the left-hand term of (1.1.4.11) remains unchanged if we interchange the indices i and j. The terms on the right-hand side therefore also remain unchanged, whatever the value of T_{ll} or T_{kl}. It follows that

$$s_{ijll} = s_{jill}$$
$$s_{ijkl} = s_{ijlk} = s_{jikl} = s_{jilk}.$$

Similar relations hold for c_{ijkl}, Q_{ijkl}, p_{ijkl} and π_{ijkl}: the submatrices **2** and **3**, **4** and **7**, **5**, **6**, **8** and **9**, respectively, are equal.

Equation (1.4.1.11) can be rewritten, introducing the coefficients of the Voigt strain matrix:

$$S_\alpha = S_{ii} = \sum_l s_{iill} T_{ll} + \sum_{k \neq l} (s_{iikl} + s_{iilk}) T_{kl} \quad (\alpha = 1, 2, 3)$$
$$S_\alpha = S_{ij} + S_{ji} = \sum_l (s_{ijll} + s_{jill}) T_{ll} + \sum_{k \neq l} (s_{ijkl} + s_{ijlk} + s_{jikl} + s_{jilk}) T_{kl} \quad (\alpha = 4, 5, 6).$$

We shall now introduce a two-index notation for the elastic compliances, according to the following conventions:

$$\left.\begin{array}{lll} i = j; & k = l; & s_{\alpha\beta} = s_{iill} \\ i = j; & k \neq l; & s_{\alpha\beta} = s_{iikl} + s_{iilk} \\ i \neq j; & k = l; & s_{\alpha\beta} = s_{ijkk} + s_{jikk} \\ i \neq j; & k \neq l; & s_{\alpha\beta} = s_{ijkl} + s_{jikl} + s_{ijlk} + s_{jilk}. \end{array}\right\} \quad (1.1.4.12)$$

We have thus associated with the fourth-rank tensor a square 6×6 matrix with 36 coefficients:

β / α	1	2	3	4	5	6
1	11	12	13	14	15	16
2	21	22	23	24	25	26
3	31	32	33	34	35	36
4	41	42	43	44	45	46
5	51	52	53	54	55	56
6	61	62	63	64	65	66

One can translate relation (1.1.4.12) using the 9×9 matrix representing s_{ijkl} by adding term by term the coefficients of submatrices **2** and **3**, **4** and **7** and **5**, **6**, **8** and **9**, respectively:

$$\left(\begin{array}{c} \mathbf{1} \\ \hline \mathbf{2+3} \end{array}\right) = \left(\begin{array}{c|c} \mathbf{1} & \mathbf{2} \\ \hline \mathbf{4+7} & \mathbf{5+6+8+9} \end{array}\right) \times \left(\begin{array}{c} \mathbf{1} \\ \hline \mathbf{2+3} \end{array}\right)$$

Using the two-index notation, equation (1.1.4.9) becomes

$$S_\alpha = s_{\alpha\beta} T_\beta. \quad (1.1.4.13)$$

A similar development can be applied to the other fourth-rank tensors π_{ijkl}, which will be replaced by 6×6 matrices with 36 coefficients, according to the following rules.

(i) *Elastic stiffnesses*, c_{ijkl} and *elasto-optic coefficients*, p_{ijkl}:

$$\left(\begin{array}{c} \mathbf{1} \\ \hline \mathbf{2} \end{array}\right) = \left(\begin{array}{c|c} \mathbf{1} & \mathbf{2} \\ \hline \mathbf{4} & \mathbf{5} \end{array}\right) \times \left(\begin{array}{c} \mathbf{1} \\ \hline \mathbf{2} \end{array}\right)$$

where

$$c_{\alpha\beta} = c_{ijkl}$$
$$p_{\alpha\beta} = p_{ijkl}.$$

(ii) *Piezo-optic coefficients*, π_{ijkl}:

$$\left(\begin{array}{c} \mathbf{1} \\ \hline \mathbf{2} \end{array}\right) = \left(\begin{array}{c|c} \mathbf{1} & \mathbf{2+3} \\ \hline \mathbf{4} & \mathbf{5+6} \end{array}\right) \times \left(\begin{array}{c} \mathbf{1} \\ \hline \mathbf{2} \end{array}\right)$$

where

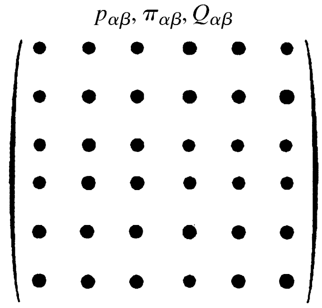
$$\left.\begin{array}{lll} i = j; & k = l; & \pi_{\alpha\beta} = \pi_{iill} \\ i = j; & k \neq l; & \pi_{\alpha\beta} = \pi_{iikl} + \pi_{iilk} \\ i \neq j; & k = l; & \pi_{\alpha\beta} = \pi_{ijkk} = \pi_{jikk} \\ i \neq j; & k \neq l; & \pi_{\alpha\beta} = \pi_{ijkl} + \pi_{jikl} = \pi_{ijlk} + \pi_{jilk}. \end{array}\right\}$$

(iii) *Electrostriction coefficients*, Q_{ijkl}: same relation as for the elastic compliances.

1.1.4.10.6. *Independent components of the matrix associated with a fourth-rank tensor according to the following point groups*

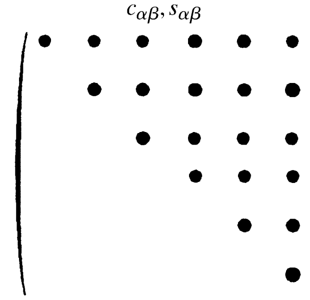
1.1.4.10.6.1. *Triclinic system, groups* $\bar{1}$, 1

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}$



36 independent components

$c_{\alpha\beta}, s_{\alpha\beta}$

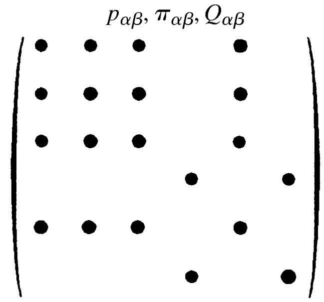


21 independent components

1.1.4.10.6.2. *Monoclinic system*

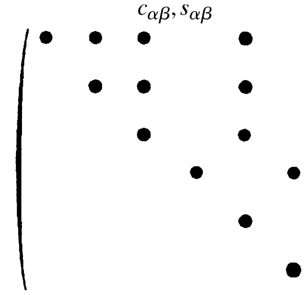
Groups $2/m$, 2, m, twofold axis parallel to Ox_2:

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}$



20 independent components

$c_{\alpha\beta}, s_{\alpha\beta}$

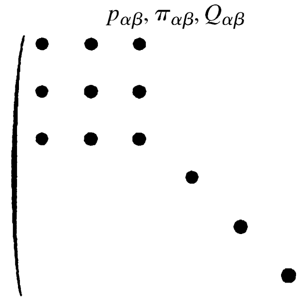


13 independent components

1.1.4.10.6.3. *Orthorhombic system*

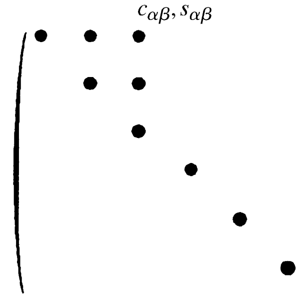
Groups mmm, $2mm$, 222:

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}$



12 independent components

$c_{\alpha\beta}, s_{\alpha\beta}$

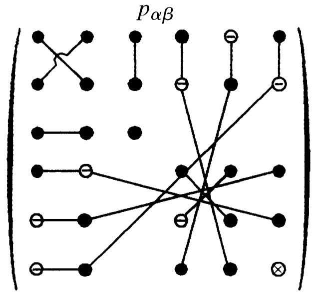


9 independent components

1.1.4.10.6.4. *Trigonal system*

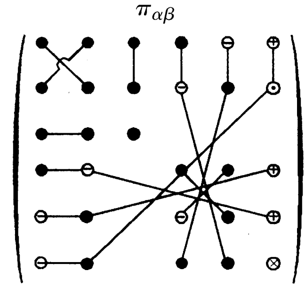
(i) Groups 3, $\bar{3}$:

$p_{\alpha\beta}$



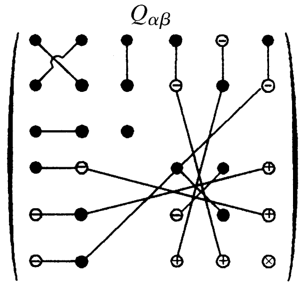
12 independent components

$\pi_{\alpha\beta}$



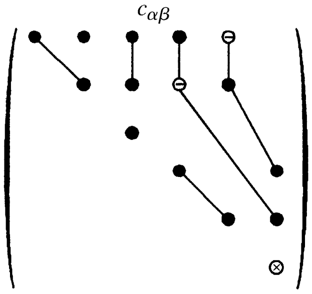
12 independent components

$Q_{\alpha\beta}$



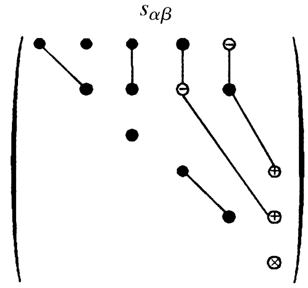
12 independent components

$c_{\alpha\beta}$



7 independent components

$s_{\alpha\beta}$

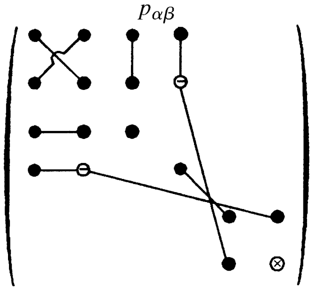


7 independent components

where ⊖ is a component numerically equal but opposite in sign to the heavy dot component to which it is linked; ⊕ is a component equal to twice the heavy dot component to which it is linked; ⊙ is a component equal to minus twice the heavy dot component to which it is linked; ⊗ is equal to $1/2(p_{11} - p_{12})$, $(\pi_{11} - \pi_{12})$, $2(Q_{11} - Q_{12})$, $1/2(c_{11} - c_{12})$ and $2(s_{11} - s_{12})$, respectively.

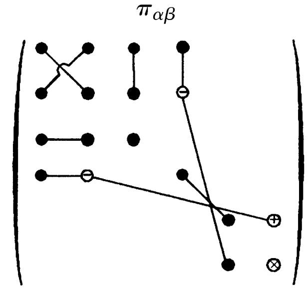
(ii) Groups 32, 3*m*, $\bar{3}m$:

$p_{\alpha\beta}$



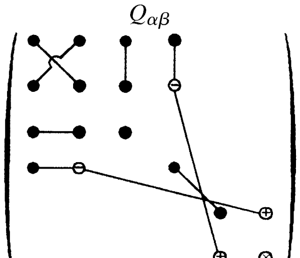
8 independent components

$\pi_{\alpha\beta}$



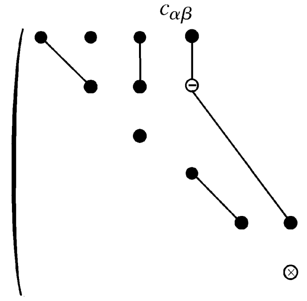
8 independent components

$Q_{\alpha\beta}$



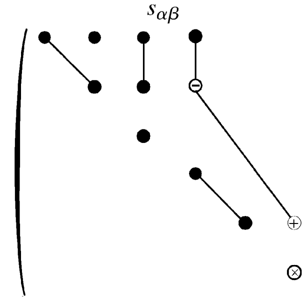
8 independent components

$c_{\alpha\beta}$



6 independent components

$s_{\alpha\beta}$



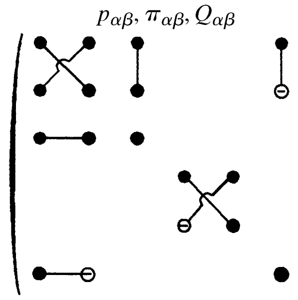
6 independent components

with the same conventions.

1.1.4.10.6.5. *Tetragonal system*

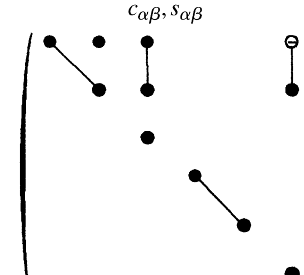
(i) Groups 4, $\bar{4}$ and $4/m$:

$p_{\alpha\beta}$, $\pi_{\alpha\beta}$, $Q_{\alpha\beta}$



10 independent components

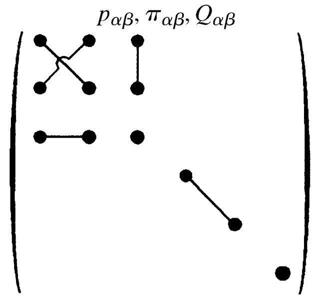
$c_{\alpha\beta}$, $s_{\alpha\beta}$



7 independent components

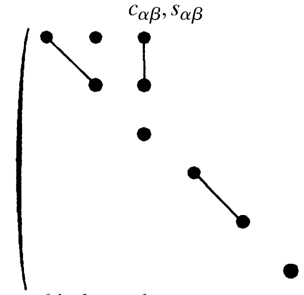
(ii) Groups 422, 4*mm*, $\bar{4}2m$ and $4/mmm$:

$p_{\alpha\beta}$, $\pi_{\alpha\beta}$, $Q_{\alpha\beta}$



7 independent components

$c_{\alpha\beta}$, $s_{\alpha\beta}$

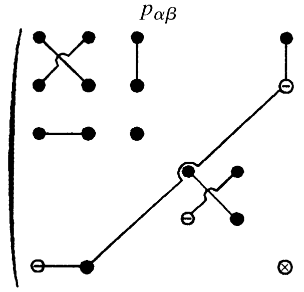


6 independent components

1.1.4.10.6.6. *Hexagonal system*

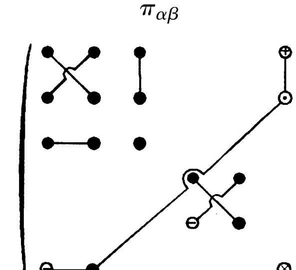
(i) Groups 6, $\bar{6}$ and $6/m$:

$p_{\alpha\beta}$



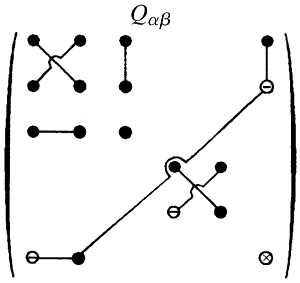
8 independent components

$\pi_{\alpha\beta}$



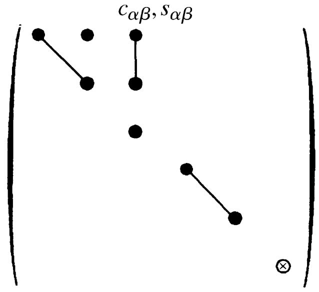
8 independent components

$Q_{\alpha\beta}$



8 independent components

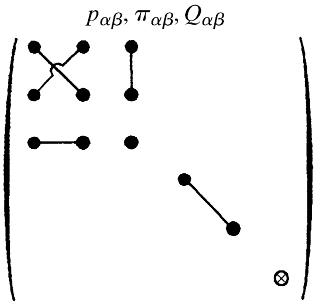
$c_{\alpha\beta}, s_{\alpha\beta}$



5 independent components

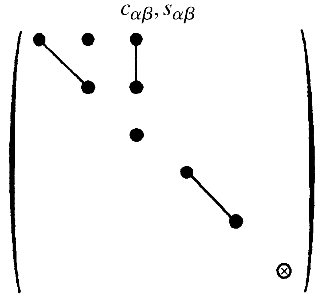
(ii) Groups 622, 6mm, $\bar{6}2m$ and 6/mm:

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}$



6 independent components

$c_{\alpha\beta}, s_{\alpha\beta}$

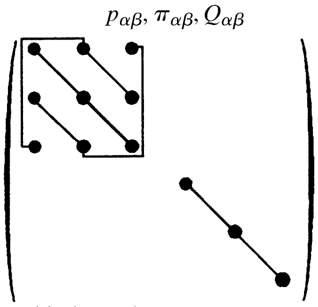


5 independent components

1.1.4.10.6.7. *Cubic system*

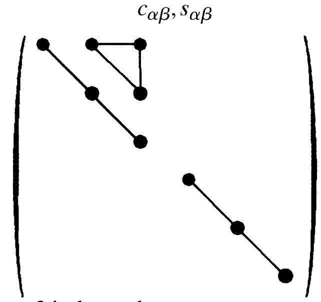
(i) Groups 23 and 3m:

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}$



4 independent components

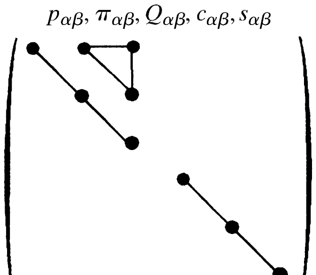
$c_{\alpha\beta}, s_{\alpha\beta}$



3 independent components

(ii) Groups 432, $\bar{4}3m$ and $m\bar{3}m$:

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}, c_{\alpha\beta}, s_{\alpha\beta}$

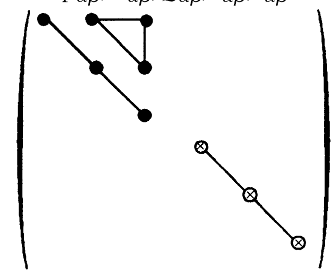


3 independent components

1.1.4.10.6.8. *Spherical system*

For all tensors

$p_{\alpha\beta}, \pi_{\alpha\beta}, Q_{\alpha\beta}, c_{\alpha\beta}, s_{\alpha\beta}$



2 independent components

1.1.4.10.7. *Reduction of the number of independent components of axial tensors of rank 2*

It was shown in Section 1.1.4.5.3.2 that axial tensors of rank 2 are actually tensors of rank 3 antisymmetric with respect to two indices. The matrix of independent components of a tensor such that

$$g_{ijk} = -g_{jik}$$

is given by

$$\left(\begin{array}{ccc|ccc|ccc} & 122 & 133 & 123 & 131 & & 132 & & 121 \\ -121 & & 223 & & 231 & -122 & 232 & -123 & \\ -131 & -232 & & -233 & & -132 & & -133 & -231 \end{array}\right).$$

The second-rank axial tensor g_{kl} associated with this tensor is defined by

$$g_{kl} = \tfrac{1}{2}\varepsilon_{ijk} g_{ijl}.$$

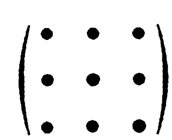
For instance, the piezomagnetic coefficients that give the magnetic moment M_i due to an applied stress T_α are the components of a second-rank axial tensor, $\Lambda_{i\alpha}$ (see Section 1.5.7.1):

$$M_i = \Lambda_{i\alpha} T_\alpha.$$

1.1.4.10.7.1. *Independent components according to the following point groups*

(i) *Triclinic system*

(a) Group 1:

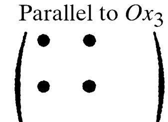


(b) Group $\bar{1}$: all components are equal to zero.

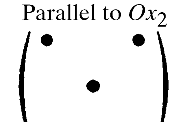
(ii) *Monoclinic system*

(a) Group 2:

Parallel to Ox_3

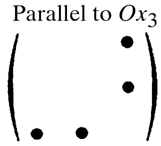


Parallel to Ox_2

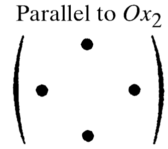


(*b*) Group *m*:

Parallel to Ox_3

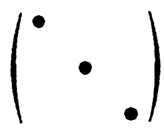


Parallel to Ox_2

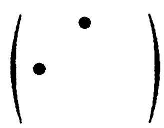


(*c*) Group $2/m$: all components are equal to zero.

(iii) *Orthorhombic system*
(*a*) Group 222:

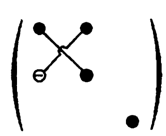


(*b*) Group *mm*2:

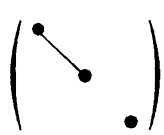


(*c*) Group *mmm*: all components are equal to zero.

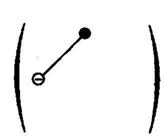
(iv) *Trigonal, tetragonal, hexagonal and cylindrical systems*
(*a*) Groups 3, 4, 6 and A_∞:



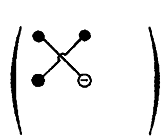
(*b*) Groups 32, 42, 62 and $A_\infty \infty A_2$:



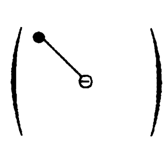
(*c*) Groups 3*m*, 4*m*, 6*m* and $A_\infty \infty M$:



(*d*) Group $\bar{4}$:

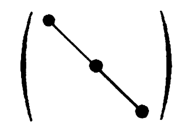


(*e*) Group $\bar{4}2m$:



(*f*) Groups $\bar{3}$, $4/m$, $\bar{6}2m$, $\bar{3}m$, $4/mm$ and $6/mm$: all components are equal to zero.

(v) *Cubic and spherical systems*
(*a*) Groups 23, 432 and ∞A_∞:



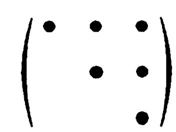
The axial tensor is reduced to a pseudoscalar.
(*b*) Groups $m\bar{3}$, $\bar{4}3m$, $m\bar{3}m$ and $\infty(A_\infty/M)C$: all components are equal to zero.

1.1.4.10.7.2. *Independent components of symmetric axial tensors according to the following point groups*

Some axial tensors are also symmetric. For instance, the optical rotatory power of a gyrotropic crystal in a given direction of direction cosines $\alpha_1, \alpha_2, \alpha_3$ is proportional to a quantity *G* defined by (see Section 1.6.5.4)

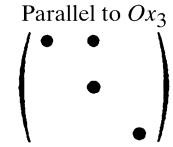
$$G = g_{ij}\alpha_i\alpha_j,$$

where the gyration tensor g_{ij} is an axial tensor. This expression shows that only the symmetric part of g_{ij} is relevant. This leads to a further reduction of the number of independent components:
(i) *Triclinic system*
(*a*) Group 1:

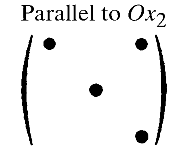


(*b*) Group $\bar{1}$: all components are equal to zero.
(ii) *Monoclinic system*
(*a*) Group 2:

Parallel to Ox_3

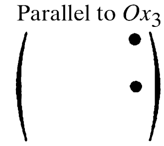


Parallel to Ox_2

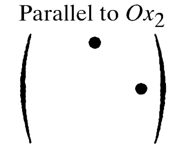


(*b*) Group *m*:

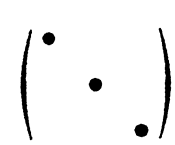
Parallel to Ox_3



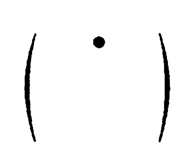
Parallel to Ox_2



(*c*) Group $2/m$: all components are equal to zero.
(iii) *Orthorhombic system*
(*a*) Group 222:



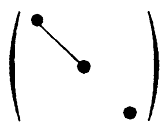
(*b*) Group *mm*2:



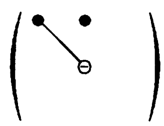
(*c*) Group *mmm*: all components are equal to zero.

(iv) *Trigonal, tetragonal and hexagonal systems*

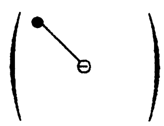
(*a*) Groups 3, 32, 4, 42, 6, 62:



(*b*) Group $\bar{4}$:



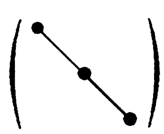
(*c*) Group $\bar{4}2m$:



(*d*) Groups $\bar{3}$, $3m$, $\bar{3}m$, $4/m$, $4mm$, $4/mm$, $\bar{6}$, $\bar{6}2m$ and $6/mm$: all components are equal to zero.

(v) *Cubic and spherical systems*

(*a*) Groups 23, 432 and $A_\infty \infty A_2$:



(*b*) Groups $m\bar{3}$, $\bar{4}3m$, $m\bar{3}m$ and $\infty(A_\infty/M)C$: all components are equal to zero.

In practice, gyrotropic crystals are only found among the enantiomorphic groups: 1, 2, 222, 3, 32, 4, 422, 6, 622, 23, 432. Pasteur (1848*a*,*b*) was the first to establish the distinction between 'molecular dissymmetry' and 'crystalline dissymetry'.

1.1.5. Thermodynamic functions and physical property tensors

[The reader may also consult Mason (1966), Nye (1985) or Sirotin & Shaskol'skaya (1982).]

1.1.5.1. *Isothermal study*

The energy of a system is the sum of all the forms of energy: thermal, mechanical, electrical *etc.* Let us consider a system whose only variables are these three. For a small variation of the associated extensive parameters, the variation of the internal energy is

$$\mathrm{d}\mathcal{U} = E_n\,\mathrm{d}D_n + T_{kl}\,\mathrm{d}S_{kl} + \Theta\,\mathrm{d}\sigma,$$

where Θ is the temperature and σ is the entropy; there is summation over all dummy indices; an orthonormal frame is assumed and variance is not apparent. The mechanical energy of deformation is given by $T_{kl}\,\mathrm{d}S_{kl}$ (see Section 1.3.2.8). Let us consider the Gibbs free-energy function $\mathcal{G}$ defined by

$$\mathcal{G} = \mathcal{U} - E_n D_n - T_{kl} S_{kl} - \Theta\sigma.$$

Differentiation of $\mathcal{G}$ gives

$$\mathrm{d}\mathcal{G} = -D_n\,\mathrm{d}E_n - S_{kl}\,\mathrm{d}T_{kl} - \sigma\,\mathrm{d}\Theta.$$

The extensive parameters are therefore partial derivatives of the free energy:

$$S_{kl} = -\frac{\partial\mathcal{G}}{\partial T_{kl}};\ \ D_n = -\frac{\partial\mathcal{G}}{\partial E_n};\ \ \sigma = -\frac{\partial\mathcal{G}}{\partial\Theta}.$$

Each of these quantities may be expanded by performing a further differentiation in terms of the intensive parameters, T_{kl}, E_n and Θ. We have, to the first order,

$$\begin{aligned}
\mathrm{d}S_{kl} &= \left[\frac{\partial S_{kl}}{\partial T_{ij}}\right]_{E,\Theta}\mathrm{d}T_{ij} + \left[\frac{\partial S_{kl}}{\partial E_n}\right]_{T,\Theta}\mathrm{d}E_n + \left[\frac{\partial S_{kl}}{\partial\Theta}\right]_{E,T}\delta\Theta\\
\mathrm{d}D_n &= \left[\frac{\partial D_n}{\partial T_{kl}}\right]_{E,\Theta}\mathrm{d}T_{kl} + \left[\frac{\partial D_n}{\partial E_m}\right]_{T,\Theta}\mathrm{d}E_m + \left[\frac{\partial D_n}{\partial\Theta}\right]_{E,T}\delta\Theta\\
\mathrm{d}\sigma &= \left[\frac{\partial\sigma}{\partial T_{ij}}\right]_{E,\Theta}\mathrm{d}T_{ij} + \left[\frac{\partial\sigma}{\partial E_m}\right]_{T,\Theta}\mathrm{d}E_m + \left[\frac{\partial\sigma}{\partial\Theta}\right]_{E,T}\delta\Theta.
\end{aligned}$$

To a first approximation, the partial derivatives may be considered as constants, and the above relations may be integrated:

$$\left.\begin{aligned}
S_{kl} &= (s_{klij})^{E,\Theta}T_{ij} + (d_{kln})^{T,\Theta}E_n + (\alpha_{kl})^{E,T}\delta\Theta\\
D_n &= (d_{nkl})^{E,\Theta}T_{kl} + (\varepsilon_{nm})^{T,\Theta}E_m + (p_n)^{E,T}\delta\Theta\\
\delta\sigma &= (\alpha_{ij})^{E}T_{ij} + (p_m)^{T}E_m + (\rho C^{E,T}/\Theta)\delta\Theta.
\end{aligned}\right\} \quad (1.1.5.1)$$

This set of equations is the equivalent of relation (1.1.1.6) of Section 1.1.1.3, which gives the coefficients of the matrix of physical properties. These coefficients are:

(i) For the principal properties: $(s_{klij})^{E,\Theta}$: elastic compliances at constant temperature and field; $(\varepsilon_{nm})^{T,\Theta}$: dielectric constant at constant temperatures and stress; $\rho C^{T,E}$: heat capacity per unit volume at constant stress and field (ρ is the specific mass and $C^{T,E}$ is the specific heat at constant stress and field).

(ii) For the other properties: $(d_{kln})^{T,\Theta}$ and $(d_{nkl})^{E,\Theta}$ are the components of the piezoelectric effect and of the converse effect. They are represented by 3×9 and 9×3 matrices, respectively. One may notice that

$$d_{kln} = \frac{\partial S_{kl}}{\partial E_n} = -\frac{\partial^2\mathcal{G}}{\partial E_n\partial T_{kl}} = -\frac{\partial^2\mathcal{G}}{\partial T_{kl}\partial E_n} = \frac{\partial D_n}{\partial T_{kl}} = d_{nkl},$$

which shows again that the components of two properties that are symmetric with respect to the leading diagonal of the matrix of physical properties are equal (Section 1.1.1.4) and that the corresponding matrices are transpose to one another.

In a similar way,

(*a*) the matrices $(\alpha_{kl})^{E,T}$ of the thermal expansion and $(\alpha_{ij})^{E}$ of the piezocalorific effect are transpose to one another;

(*b*) the components $(p_n)^{T}$ of the pyroelectric and of the electrocalorific effects are equal.

Remark. The piezoelectric effect, namely the existence of an electric polarization **P** under an applied stress, is always measured at zero applied electric field and at constant temperature. The second equation of (1.1.5.1) becomes under these circumstances

$$P_n = D_n = (d_{nkl})^{\Theta}T_{kl}.$$

Remark. Equations (1.1.5.1) are, as has been said, first-order approximations because we have assumed the partial derivatives to be constants. Actually, this approximation is not correct, and in many cases it is necessary to take into account the higher-order terms as, for instance, in:

(*a*) nonlinear elasticity (see Sections 1.3.6 and 1.3.7);

(*b*) electrostriction;

(*c*) nonlinear optics (see Chapter 1.7);

(*d*) electro-optic and piezo-optic effects (see Sections 1.6.6 and 1.6.7).