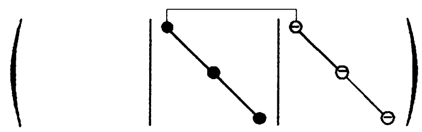
International Tables for Crystallography (2006). Vol. D, Section 1.1.4.9, pp. 20–24.

1.1.4.8.7.2. *Groups* 432 *and* $\infty A_\infty/M$

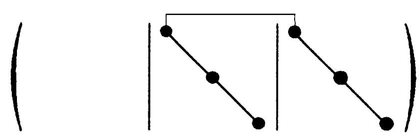
One combines the reductions corresponding to groups 422 and 23:



There is 1 independent component.

1.1.4.8.7.3. *Group* $\bar{4}3m$

One combines the reductions corresponding to groups $\bar{4}2m$ and 23:



There is 1 independent component.

1.1.4.8.7.4. *Groups* $m\bar{3}$, $m\bar{3}m$ *and* $\infty(A_\infty/M)C$

All the components are equal to zero.

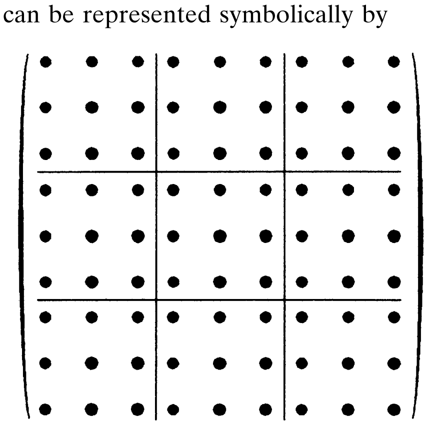
1.1.4.9. *Reduction of the components of a tensor of rank 4*

1.1.4.9.1. *Triclinic system (groups* $\bar{1}$, 1*)*

There is no reduction; all the components are independent. Their number is equal to 81. They are usually represented as a 9×9 matrix, where components t_{ijkl} are replaced by *ijkl*, for brevity:

kl / *ij*	11	22	33	23	31	12	32	13	21
11	1111	1122	1133	1123	1131	1112	1132	1113	1121
22	2211	2222	2233	2223	2231	2212	2232	2213	2221
33	3311	3322	3333	3323	3331	3312	3332	3313	3321
23	2311	2322	2333	2323	2331	2312	2332	2313	2321
31	3111	3122	3133	3123	3131	3112	3132	3113	3121
12	1211	1222	1233	1223	1231	1212	1232	1213	1221
32	3211	3222	3233	3223	3231	3212	3232	3213	3221
13	1311	1322	1333	1323	1331	1312	1332	1313	1321
21	2111	2122	2133	2123	2131	2112	2132	2113	2121

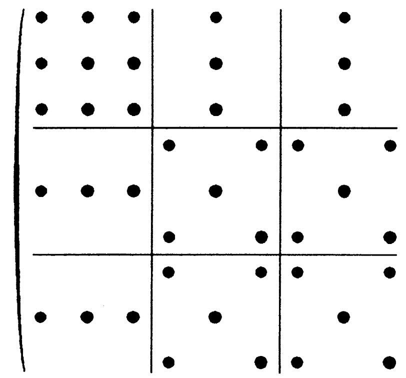
This matrix can be represented symbolically by



where the 9×9 matrix has been subdivided for clarity in to nine 3×3 submatrices.

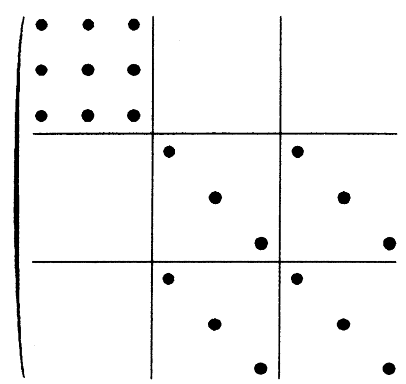
1.1.4.9.2. *Monoclinic system (groups* $2/m$, 2, m*)*

The reduction is obtained by the method of direct inspection. For a twofold axis parallel to Ox_2, one finds



There are 41 independent components.

1.1.4.9.3. *Orthorhombic system (groups mmm,* 2*mm,* 222*)*



There are 21 independent components.

1.1.4.9.4. *Trigonal system*

1.1.4.9.4.1. *Groups* 3 *and* $\bar{3}$

The reduction is first applied in the system of axes tied to the eigenvectors of the operator representing a threefold axis. The system of axes is then changed to a system of orthonormal axes with Ox_3 parallel to the threefold axis:

kl / *ij*	11	22	33	23	31	12	32	13	21
11	1111	1122	1133	1123	−2231	1112	1132	−2213	1121
22	1122	1111	1133	−1123	2231	−1121	−1132	2213	−1112
33	3311	3311	3333			3312			−3312
23	2311	−2311		2323	2331	1322	2332	2313	1322
31	−3122	3122		3123	3131	3211	3132	3113	3211
12	1211	−2111	1233	2213	1132	1212	2231	1123	1221
32	3211	−3211		3113	−3132	3122	3131	−3123	3122
13	−1322	1322		−2313	2332	2311	−2331	2323	2311
21	2111	−121	−1233	2213	1132	1221	2231	1123	1212

with

$$\left.\begin{aligned} t_{1111} - t_{1122} &= t_{1212} + t_{1221} \\ t_{1112} + t_{1121} &= -(t_{1211} + t_{2111}). \end{aligned}\right\}$$

There are 27 independent components.

1.1.4.9.4.2. *Groups* $\bar{3}m$, 32, 3*m*, *with the twofold axis parallel to* Ox_1

ij \ *kl*	11	22	33	23	31	12	32	13	21
11	1111	1122	1133	1123			1132		
22	1122	1111	1133	−1123			−1132		
33	3311	3311	3333						
23	2311	−2311		2323			2332		
31					3131	3211		3113	3211
12					1132	1212		1123	1221
32	3211	−3211		3113			3131		
13					2332	2311		2323	2311
21					1132	1221		1123	1212

with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 14 independent components.

1.1.4.9.5. *Tetragonal system*

1.1.4.9.5.1. *Groups* 4/*m*, 4, $\bar{4}$

ij \ *kl*	11	22	33	23	31	12	32	13	21
11	1111	1122	1133			1112			−2212
22	1122	1111	1133			2212			−1112
33	3311	3311	3333			3312			−3312
23				2323	2331		2332	2313	
31				3123	3131		3132	3113	
12	1211	1222	1233			1212			1221
32				3113	−3132		3131	−3123	
13				−2313	2332		−2331	2323	
21	−1222	−1211	−1233						1212

There are 21 independent components.

1.1.4.9.5.2. *Groups* 4/*mm*, 422, 4*mm*, $\bar{4}2m$

ij \ *kl*	11	22	33	23	31	12	32	13	21
11	1111	1122	1133						
22	1122	1111	1133						
33	3311	3311	3333						
23				2323			2332		
31					3131			3113	
12						1212			1221
32				3113			3131		
13					2332			2323	
21						1221			1212

There are 11 independent components.

1.1.4.9.6. *Hexagonal and cylindrical systems*

1.1.4.9.6.1. *Groups* 6/*m*, $\bar{6}$, 6; $(A_\infty/M)C$, A_∞

ij \ *kl*	11	22	33	23	31	12	32	13	21
11	1111	1122	1133			1112			1121
22	1122	1111	1133			−1121			−1112
33	3311	3311	3333			3312			−3312
23				2323	2331		2332	2313	
31				3123	3131		3132	3113	
12	1211	−2111	1233			1212			1221
32				3113	−3132		3131	−3123	
13				−2313	2332		−2331	2323	
21	2111	−1211	−1233		1132	1221		1123	1212

with

$$\left.\begin{aligned} t_{1111} - t_{1122} &= t_{1212} + t_{1221} \\ t_{1112} + t_{1121} &= -(t_{1211} + t_{2111}). \end{aligned}\right\}$$

There are 19 independent components.

1.1.4.9.6.2. *Groups* 6/*mm*, 622, 6*mm*, $\bar{6}2m$; $(A_\infty/M)\infty$; $(A_2/M)C$, $A_\infty \infty A_2$

ij \ *kl*	11	22	33	23	31	12	32	13	21
11	1111	1122	1133						
22	1122	1111	1133						
33	3311	3311	3333						
23				2323			2332		
31					3131			3113	
12						1212			1221
32				3113			3131		
13					2332			2323	
21						1221			1212

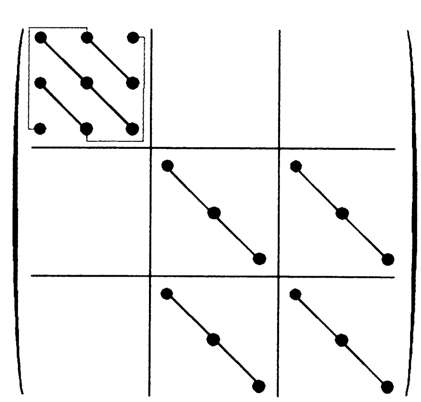
with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 11 independent components.

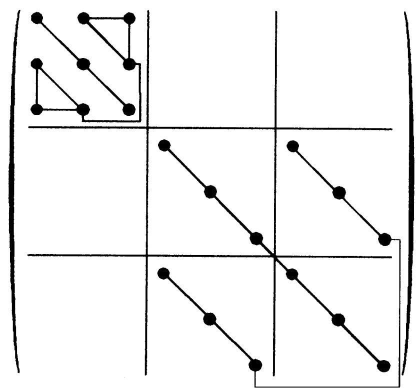
1.1.4.9.7. *Cubic system*

1.1.4.9.7.1. *Groups* 23, $\bar{3}m$



There are 7 independent components.

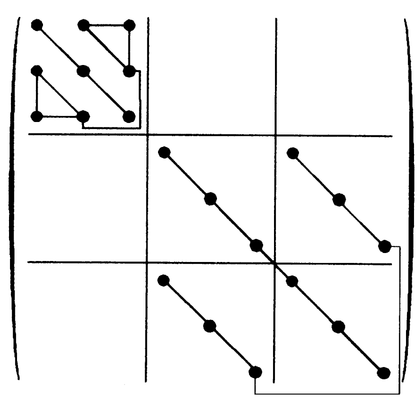
1.1.4.9.7.2. *Groups* $m\bar{3}m$, 432, $\bar{4}3m$



There are 4 independent components. The tensor is symmetric.

1.1.4.9.8. *Spherical system*

1.1.4.9.8.1. *Groups* $\infty(A_\infty/M)C$ *and* ∞A_∞



with

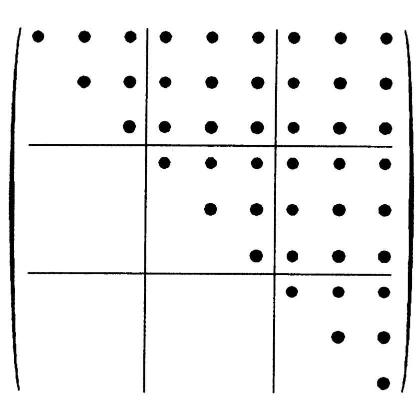
$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 3 independent components. The tensor is symmetric.

1.1.4.9.9. *Symmetric tensors of rank 4*

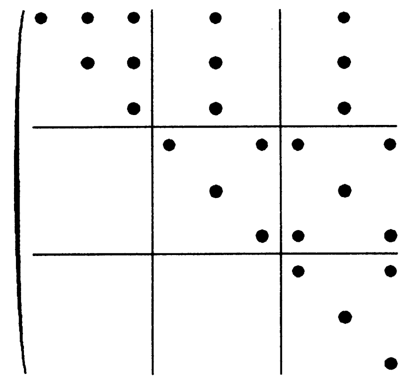
For symmetric tensors such as those representing principal properties, one finds the following, representing the nonzero components for the leading diagonal and for one half of the others.

1.1.4.9.9.1. *Triclinic system*



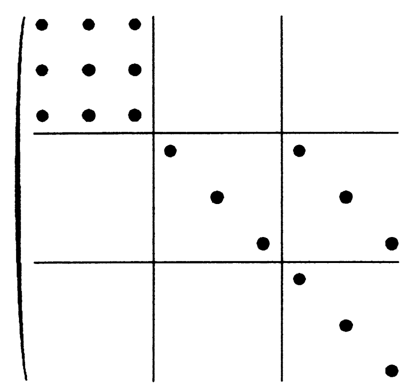
There are 45 independent coefficients.

1.1.4.9.9.2. *Monoclinic system*



There are 25 independent coefficients.

1.1.4.9.9.3. *Orthorhombic system*



There are 15 independent coefficients.

1.1.4.9.9.4. *Trigonal system*

(i) Groups 3 and $\bar{3}$

kl / *ij*	11	22	33	23	31	12	32	13	21
11	1111	1122	1133	1123	−2231	1112	1132	−2213	−1112
22		1111	1133	−1123	2231	−1121	−1132	2213	−1112
33			3333			3312			−3312
23				2323	2331	2213	2332		2213
31					3131	1132		2332	1132
12						1212	2231	1123	1221
32							3131	−2331	2231
13								2323	1123
21									1212

with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 15 independent components.

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

ij \ kl	11	22	33	23	31	12	32	13	21
11	1111	1122	1133	1123			1132		
22		1111	1133	−1123			−1132		
33			3333						
23				2323			2332		
31					3131	1132		2332	1132
12						1212		1123	1221
32							3131		
13								2323	1123
21									1212

with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 11 independent components.

1.1.4.9.9.5. *Tetragonal system*

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

ij \ kl	11	22	33	23	31	12	32	13	21
11	1111	1122	1133			1112			−2212
22		1111	1133			2212			−1112
33			3333			3312			−3312
23				2323	2331		2332		
31					3131			2332	
12						1212			1221
32							3131	−2331	
13								2323	
21									1212

There are 13 independent components.

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

ij \ kl	11	22	33	23	31	12	32	13	21
11	1111	1122	1133						
22		1111	1133						
33			3333						
23				2323			2332		
31					3131			3113	
12						1212			1221
32							3131		
13								2323	
21									1212

There are 9 independent components.

1.1.4.9.9.6. *Hexagonal and cylindrical systems*

(i) Groups $6/m$, $\bar{6}$, 6; $(A_\infty/M)C$, A_∞

ij \ kl	11	22	33	23	31	12	32	13	21
11	1111	1122	1133			1112			1121
22		1111	1133			−1121			−1112
33			3333			3312			−3312
23				2323	2331		2332		
31					3131		3132	2332	
12						1212			1221
32							3131	−2331	
13								2323	
21									1212

with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 12 independent components.

(ii) Groups $6/mm$, 622, 6mm, $\bar{6}2m$; $(A_\infty/M)\infty(A_2/M)C$, $A_\infty\infty A_2$

ij \ kl	11	22	33	23	31	12	32	13	21
11	1111	1122	1133						
22		1111	1133						
33			3333						
23				2323			2332		
31					3131			3113	
12						1212			1221
32							3131		
13								2323	
21									1212

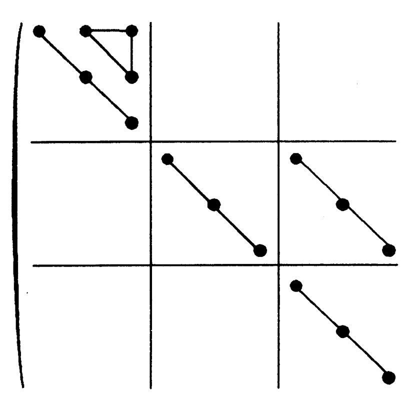
with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 10 independent components.

1.1.4.9.9.7. *Cubic system*

(i) Groups 23, $\bar{3}m$



with

$$t_{1111} - t_{1122} = t_{1212} + t_{1221}.$$

There are 5 independent components.

(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):

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

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 $E_k E_l$, 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:

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

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**:

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

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:

references