

## 12

### Appendix

#### 12.1

##### List of Common Symbols

(multiple meanings possible!)

$\alpha_i$	Angle of the crystallographic metric
$a_i$	Length of crystallographic basis vectors
$a_{ij}$	Components of the polarization tensor
$\alpha_{ij}$	Components of the tensor of thermal expansion
$B_i$	Components of the magnetic induction vector
$C_V, C_p$	Specific heats at constant volume and constant hydrostatic pressure
$c$	Speed of light in vacuum
$c_{ijkl}, c_{ij}$	Components of the elastic tensor or elastic constants
$\delta_{ij}$	Kronecker symbol
$d_{ijk}$	Components of the piezoelectric tensor
$\hat{d}_{ijk}$	Components of the electrostrictive tensor
$D_i$	Components of the dielectric displacement vector
$\epsilon_{ij}$	Components of the dielectricity tensor
$\epsilon_0$	Vacuum permittivity ( $8.8542 \cdot 10^{-12} \text{ C V}^{-1} \text{ m}^{-1}$ )
$\varepsilon_{ij}$	Components of the deformation tensor
$E_i$	Components of the electric field vector
$e_{ijk}$	Components of the piezoelectric $e$ tensor or the Levi-Civita tensor
$F$	Abrasive strength or Helmholtz energy
$\gamma_{ij}$	Components of the Grüneisen tensor
$G$	Gibbs energy
$g_i$	Components of the normalized propagation vector
$g_{ijk}$	Components of the gyration tensor
$g_{ijkl}$	Components of the electrogyration tensor
$H_i$	Components of the magnetic field vector

$h$	Planck constant ( $6.6262 \cdot 10^{-34}$ J s)
$h_i$	Miller indices
$I_i$	Components of the electric current density vector
$k$	Boltzmann constant ( $1.380662 \cdot 10^{-23}$ J K <sup>-1</sup> )
$K$	Volume compressibility
$k_i$	Components of the propagation vector
$K_i$	Components of a force vector
$\kappa_{ij}$	Components of the magnetic susceptibility vector
$k_t$	electromechanical coupling constant for a longitudinal thickness vibration
$\lambda$	Wavelength
$\lambda_{ij}$	Components of the thermal conductivity tensor
$L$	Transmission path length
$\mu_{ij}$	Components of the magnetic permeability tensor
$\mu_0$	Vacuum permeability ( $4\pi \cdot 10^{-7}$ V s A <sup>-1</sup> m <sup>-1</sup> )
$\nu$	Frequency
$n_i$	Principal refractivities
$\pi_i$	Components of the pyroelectric tensor
$p$	Hydrostatic pressure
$P_{ij} = dc_{ij}/dp$	Piezoelastic constants
$p_{ijkl}$	Components of the elasto-optic tensor
$Q_i$	Components of the heat flow density vector
$q_{ijkl}$	Components of the piezo-optic tensor
$\rho$	Density
$r_{ijk}, r_{ijkl}$	Components of the first-and second-order electro-optic tensor
$\sigma_{ij}$	Components of the mechanical strain tensor
$S$	Entropy
$s_{ij}$	Elastic coefficients or components of the electrical conductivity tensor
$s_{ijkl}$	Components of the elastic $s$ tensor
$t$	Time
$T$	Temperature
$T_{ij} = \frac{d \log c_{ij}}{dT}$	thermoelastic constants
$V$	Volume
$U$	Internal Energy
$v$	Velocity of light or sound
$\omega = 2\pi\nu$	Angular frequency

## 12.2

**Systems of Units, Units, Symbols and Conversion Factors**

The continuing use of several systems of units has created substantial confusion particularly among beginners and laymen. The introduction of the SI system (Système International d'Unités) in 1960 has reduced this confusion to some extent. Today, the use of SI-compliant units, of which some are collected in Table 12.1, is strongly recommended. The definition of the base units is assumed to be known and will not be repeated here. Prefixes that may be used with a unit to indicate decimal multiples and submultiples are (symbol in parantheses):

$10^{12}$ :	tera	(T)	$10^{-1}$ :	deci	(d)
$10^9$ :	giga	(G)	$10^{-2}$ :	centi	(c)
$10^6$ :	mega	(M)	$10^{-3}$ :	milli	(m)
$10^3$ :	kilo	(k)	$10^{-6}$ :	micro	( $\mu$ )
$10^2$ :	hecto	(h)	$10^{-9}$ :	nano	(n)
$10^1$ :	deka	(d)	$10^{-12}$ :	pico	(p)

A number of outdated units are still encountered; their use is, however, not recommended. Some examples are:

Force	:	$1 \text{ dyn} = 10^{-5} \text{ N}$
Pressure	:	$1 \text{ bar} = 10^5 \text{ Pa} = 10^5 \text{ N m}^{-2}$
Density	:	$1 \text{ g cm}^{-3} = 10^3 \text{ kg m}^{-3}$
Energy	:	$1 \text{ erg} = 10^{-7} \text{ J},$
	:	$1 \text{ cal} = 4.187 \text{ J},$
	:	$1 \text{ kWh} = 3.6 \cdot 10^6 \text{ J},$
	:	$1 \text{ eV} = 1.602 \cdot 10^{-19} \text{ J}$
Charge	:	$1 \text{ esu} = \frac{1}{3} \cdot 10^{-9} \text{ C}$

In some disciplines, the cgs system of units is still in use. For mechanical units, the conversion factors to SI units are always simple powers of ten. This is different for electric and magnetic quantities, where more complex factors arise because of the respective definitions of electrical charge in the different measurement systems. The conversion into other units thus requires particular care. To avoid these difficulties, the exclusive use of SI units is strongly recommended especially for electric and magnetic quantities. For theoretical derivations, however, the choice of a different measurement system may be appropriate if this allows for a more concise mathematical description; we have also taken this liberty in a few cases in this text.

The derived units for elastic, piezoelectric, electrooptical or magneto-optical quantities can be determined without difficulty. Some interesting remarks regarding units are given in *Pure and Applied Chemistry*, Vol. 21, pp. 1–113 (1970).

**Table 12.1** SI units.

Quantity	Unit	Symbol
Length	meter	m
Area	square meter	m <sup>2</sup>
Volume	cubic meter	m <sup>3</sup>
Plane angle	degree or radian	° or rad ( $360^\circ = 2\pi$ rad)
Solid angle	steradian	sr
Mass	kilogram	kg
Density	kilogram per cubic meter	kg m <sup>-3</sup>
Time	second	s
Frequency	hertz (one cycle per second)	Hz
Speed, velocity	meter per second	m s <sup>-1</sup>
Acceleration	meter per second squared	m s <sup>-2</sup>
Force	newton	N
Pressure, mech. stress	pascal	Pa ( $1 \text{ Pa} = 1 \text{ N m}^{-2}$ )
Energy	joule	J ( $1 \text{ J} = 1 \text{ N m}$ )
Power	watt	W ( $1 \text{ W} = 1 \text{ J s}^{-1} = 1 \text{ N m s}^{-1}$ )
Electric potential	volt	V
Resistance	ohm	$\Omega$
Charge	coulomb	C
Electric displacement	coulomb per square meter	C m <sup>-2</sup>
Electric current	ampère	A
Capacitance	farad	F
Electric field strength	volt per meter	V m <sup>-1</sup>
Magnetic flux	weber	Wb
Magnetic induction	tesla	T
Magnetic field strength	ampère per meter	A m <sup>-1</sup>
Inductance	henry	H
Temperature	kelvin (degree centigrade)	K (°C) ( $T/\text{K} = 273.15 + T/^\circ\text{C}$ )

### 12.3

#### Determination of the Point Space Group of a Crystal From Its Physical Properties

Group A: acentric PSG (1, 2, m, 22, mm, 3, 32, 3m, 4, 42, 4m,  $\bar{4}$ ,  $\bar{4}2$ , 6, 62, 6m,  $\bar{6}$ ,  $\bar{6}2$ , 23, 43,  $\bar{4}3$ );

Group B: centrosymmetric PSG ( $\bar{1}$ , 2/m, mmm,  $\bar{3}$ ,  $\bar{3}m$ , 4/m, 4/mm, 6/m, 6/mm, m3, 4/m3).

A preliminary investigation of a crystalline powder using optical frequency doubling (SHG test, see Section 4.4.4) and the piezoelectric effect (Giebe–Scheibe method, see Section 4.4.1) or the longitudinal piezoelectric effect (micro-miniaturized for small crystals) yields the classification of a crystal structure into group A or B except for the PSG 42, 62, and 43, provided the observed effects are large enough.

Investigations using polarization microscopy enable the classification into the following groups:

	A:	B:
optically isotropic	23, 43, $\bar{4}3$	$m\bar{3}$ , $4/m\bar{3}$
optically uniaxial	3, 32, 3m, 4, 42, 4m $\bar{4}$ , $\bar{4}2$ , 6, 62, 6m, $\bar{6}$ , $\bar{6}2$	$\bar{3}$ , $\bar{3}m$ , $4/m$ , $4/mm$ , $6/m$ , $6/mm$
optically biaxial	1, 2, m, 22, mm	$\bar{1}$ , $2/m$ , mmm

Crystals from group A can be further classified according to their optical activity. Cubic crystals display optical activity only in PSG 23 and 43. In 1, 2, 22, 3, 32, 4, 42, 6, and 62, a rotation of the plane of polarization along the optical axis is observed.

Other properties that can be described by polar tensors of rank two, such as thermal expansion, thermal conductivity, dielectric properties, exhibit the same symmetry as the optical properties.

A pyroelectric effect can occur in the following PSG of group A: 1, 2, m, mm, 3, 3m, 4, 4m, 6, 6m.

The form of the piezoelectric (or electrooptic) tensor allows a unique determination of the PSG of acentric crystals, except for PSG 43 (no effect) and the pairs 42 and 62, 4m and 6m, 23 and  $\bar{4}3m$ , which cannot be distinguished. If one analyzes, in addition, the elastic properties, the pairs 42 and 62 as well as 4m and 6m can be distinguished, but not 23 and  $\bar{4}3$ . Crystals from group B (Laue groups) can be distinguished from their elastic properties, with the exception of  $6/m$  and  $6/mm$ , and  $m\bar{3}$  and  $4/m\bar{3}$ . The pairs 23 and  $\bar{4}3$ ,  $m\bar{3}$  and  $4/m\bar{3}$ ,  $6/m$  and  $6/mm$  can be distinguished macroscopically only with the aid of certain 4th-rank tensors (such as the piezooptic effect, electrogyration, or 2nd-order electrostriction). The PSG 43 and  $4/m\bar{3}$  can best be distinguished from an analysis of their optical activity. If this provides no clear distinction, higher-order effects must be employed. Note, however, that all properties that are described by tensors of even rank can at most indicate to which of the eleven Laue groups the crystal belongs.

This procedure can in most cases be avoided, however, by analyzing the morphological properties (particularly spherical growth and etching tests) and diffractograms (particularly Laue diagrams). Also, a complete structure determination provides almost always a clear indication of the space group and the PSG of the investigated crystal.

## 12.4

## Electric and Magnetic Effects and Properties up to 4th-Rank Tensors

See Tables 12.2 and 12.3.

**Table 12.2** Electric and magnetic effects.  $D$  electric displacement,  $E$  electric field strength,  $B$  magnetic induction,  $H$  magnetic field strength,  $I$  electric current density,  $T$  temperature,  $\{\varepsilon_{ij}\}$  tensor of mechanical deformation,  $\{\sigma_{ij}\}$  tensor of mechanical stress. In place of the relations used here with independent quantities  $E, H, \sigma$ , and  $T$ , corresponding relations between  $D, B$ , and  $\varepsilon$  as inducing quantities can also be used in many cases. p: polar tensor, a: axial tensor.

Quantity	Electric phenomena	Type
Pyroelectricity	$\Delta P_i = \pi_i \Delta T$	p
Dielectric susceptibility	$D_i = \epsilon_{ij} E_j = \epsilon_0 (\delta_{ij} + \kappa_{ij}) E_j$	p
Magnetoelectric susceptibility	$D_i = \alpha_{ij} H_j$	a
Electric conductivity	$I_i = s_{ij} E_j$	p
Piezoelectricity	$P_i = d_{ijk} \sigma_{jk}$	p
1st-order electrostriction	$\varepsilon_{ij} = \tilde{d}_{ijk} E_k$	p
1st-order nonlinear dielectric susceptibility	$D_i = \epsilon_{ijk} E_j E_k$	p
1st-order electrooptic effect (Pockels)	$\Delta a_{ij} = r_{ijk} E_k$	p
Optical activity	$D_i = \epsilon_{ij} E_j + g_{ijk} \frac{\partial E_j}{\partial x_k}$ ( $g_{ijk} = -g_{jik}$ )	p
1st-order magnetoelectric effect	$D_i = \gamma_{ijk} H_j E_k$	a
1st-order electric resistance change	$\Delta s_{ij} = s_{ijk} E_k$	p
2nd-order magnetoelectric susceptibility	$D_i = \alpha_{ijk} H_j H_k$	p
Hall effect	$E_i = k_{ijk} I_j H_k$	a
2nd-order electrostriction	$\varepsilon_{ij} = \tilde{d}_{ijkl} E_k E_l$	p
2nd-order electric resistance change	$\Delta s_{ij} = s_{ijkl} E_k E_l$	p
Magnetoelectrostriction	$\varepsilon_{ij} = v_{ijkl} H_k E_l$	a
2nd-order nonlinear dielectric susceptibility	$D_i = \epsilon_{ijkl} E_j E_k E_l$	p
higher-order magnetoelectric effects	$D_i = u_{ijkl} H_j E_k E_l$	a
higher-order magnetoelectric effects	$D_i = \gamma_{ijkl} H_j H_k E_l$	p
higher-order magnetoelectric effects	$D_i = \alpha_{ijkl} H_j H_k H_l$	a
Electrically induced piezoelectricity	$P_i = {}^e d_{ijkl} E_j \sigma_{kl}$	p
Electrically induced optical activity (electrogyration)	$D_i = g_{ijkl} E_j \frac{\partial E_k}{\partial x_l}$	p
Magnetically induced piezoelectricity	$P_i = {}^m d_{ijkl} H_j \sigma_{kl}$	a
2nd-order electrooptic effect (Kerr effect)	$\Delta a_{ij} = r_{ijkl} E_k E_l$	p
Magnetoelectrooptic effect	$\Delta a_{ij} = n_{ijkl} H_k E_l$	a
2nd-order piezoelectricity	$P_i = \dots + d_{ijklm} \sigma_{jk} \sigma_{lm}$	p

**Table 12.3** Electric and magnetic effects (continued from Table 12.2).

Quantity	Magnetic phenomena	Type
Pyromagnetism	$\Delta B_i = \beta_i \Delta T$	a
Magnetic susceptibility	$B_i = \mu_{ij} H_j = \mu_0 (\delta_{ij} + \kappa_{ij}) H_j$	p
Electromagnetic susceptibility	$B_i = \beta_{ij} E_j$	a
Piezomagnetism	$B_i = q_{ijk} \sigma_{jk}$	a
1st-order magnetostriction	$\varepsilon_{ij} = f_{ijk} H_k$	a
Nonlinear magnetic susceptibility	$B_i = \mu_{ijk} H_j H_k$	a
1st-order magnetooptic effect	$\Delta a_{ij} = m_{ijk} H_k$	a
Faraday effect	$D_i = \epsilon_{ij} E_j + z_{ijk} E_j H_k$ ( $z_{ijk} = -z_{jik}$ )	a
1st-order electromagnetic effect	$B_i = \eta_{ijk} E_j H_k$	p
1st-order magnetic resistance change	$I_i = s_{ij} E_j + t_{ijk} E_j H_k$ $\Delta s_{ij} = t_{ijk} H_k$	a
2nd-order electromagnetic susceptibility	$B_i = \beta_{ijk} E_j E_k$	a
2nd-order magnetostriction	$\varepsilon_{ij} = f_{ijkl} H_k H_l$	p
Magnetoelectric resistance change	$\Delta s_{ij} = w_{ijkl} H_k E_l$	a
2nd-order magnetic resistance change	$\Delta S_{ij} = u_{ijkl} H_k H_l$	p
2nd-order nonlinear magnetic susceptibility	$B_i = \mu_{ijkl} H_j H_k H_l$	a
higher-order electromagnetic effects	$B_i = \eta_{ijkl} E_j H_k H_l$	a
higher-order electromagnetic effects	$B_i = \zeta_{ijkl} E_j E_k H_l$	p
higher-order electromagnetic effects	$B_i = \beta_{ijkl} E_j E_k E_l$	a
Magnetically induced piezomagnetism	$B_i = {}^m q_{ijkl} H_j \sigma_{kl}$	p
Magnetically induced optical activity (electrogyration)	$D_i = {}^m g_{ijkl} H_j \frac{\partial E_k}{\partial x_l}$	a
Electrically induced piezomagnetism	$B_i = {}^e q_{ijkl} E_j \sigma_{kl}$	a
2nd-order magnetooptic effect (Cotton-Mouton-Effekt)	$\Delta a_{ij} = m_{ijkl} H_k H_l$	p
2nd-order piezomagnetism	$B_i = \dots + q_{ijklm} \sigma_{jk} \sigma_{lm}$	a

12.5

Tables of Standard Values

Data for more crystals can be obtained from the tables in “Landolt–Börnstein”. Digits in parentheses indicate error intervals for the last digit given. All values are for approximately 293 K and standard pressure. Where the PSG is not indicated, the crystal is cubic.

Table 12.4 Density and specific heat.

	Density $\rho$ [g cm <sup>-3</sup> ]	Specific heat $C_p$ [J g <sup>-1</sup> K <sup>-1</sup> ]
Diamond	3.5150(3)	0.511
Si	2.3283(2)	0.712
LiF	2.6406(2)	1.616
NaCl	2.1644(2)	0.870
CaF <sub>2</sub>	3.1804(4)	0.912
KAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	1.7530(3)	1.47
CsAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	1.9995(3)	1.09
$\alpha$ -Quartz (32)	2.6481(3)	0.744
Calcite (CaCO <sub>3</sub> ) ( $\bar{3}m$ )	2.7102(3)	0.829
Quartz glass (Spectrosil)	2.200(1)	0.73(2)
Air (dry)	0.00121(1)	1.02(1)

Table 12.5 Pyroelectric effect.

	$\pi_i^\sigma$ [ $\mu\text{C m}^{-2}\text{K}^{-1}$ ]
Turmaline (3m)	$\pi_3^\sigma = 4.3$
Li <sub>2</sub> GeO <sub>3</sub> (mm2)	$\pi_3^\sigma = -21.4$
(CH <sub>2</sub> NH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> SO <sub>4</sub> , TGS (2)	$\pi_2^\sigma = 350$
(CH <sub>2</sub> NH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> SeO <sub>4</sub> (2)	$\pi_2^\sigma = 4200$
BaTiO <sub>3</sub> (4m)	$\pi_3^\sigma = 280$

Table 12.6 Relative permittivities of non-ferroelectric crystals at about 10 MHz at constant mechanical stress.

	$\epsilon_{\text{rel},11}$
LiF	9.036(4)
NaCl	5.895(2)
CaF <sub>2</sub>	6.799(2)
KAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	6.55(5)
CsAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	5.50(5)
$\alpha$ -Quartz (32)	$\epsilon_{\text{rel},11} = 4.520(2)$ , $\epsilon_{\text{rel},33} = 4.640(2)$



**Table 12.7** Relative permittivities of ferroelectric crystals at about 1 kHz close to the Curie temperature  $T_c$ . The asterisk \* denotes the direction of the ferroelectric polarization  $P_s$ .

	$T_c$ [K]	$\epsilon_{\text{rel},11}$	$\epsilon_{\text{rel},22}$	$\epsilon_{\text{rel},33}$	$P_s$ [ $10^4 \mu\text{Cm}^{-2}$ ]
$\text{NaKC}_4\text{H}_4\text{O}_6 \cdot 4\text{H}_2\text{O}$	297	$\approx 3 \cdot 10^3^*$	$\approx 8.8$	$\approx 9.4$	0.25
(Seignette salt, $22 \rightarrow 2$ and $2 \rightarrow 22$ ) <sup>1</sup>	255	$\approx 3 \cdot 10^3^*$	$\approx 8.8$	$\approx 9.4$	
$(\text{CH}_2\text{NH}_2\text{COOH})_3 \cdot \text{H}_2\text{SO}_4$ (TGS, $2/m \rightarrow 2$ )	322	$\approx 9.0$	$\approx 5 \cdot 10^5^*$	$\approx 8$	2.8
$\text{BaTiO}_3$ ( $4/m3 \rightarrow 4m$ )	408	$\approx 10^4$	$\approx 10^4$	$\approx 10^4^*$	26.0
$\text{KH}_2\text{PO}_4$ (KDP, $\bar{4}2 \rightarrow m2$ )	123	$\approx 50$	$\approx 50$	$\approx 10^5^*$	4.75

<sup>1</sup> Seignette salt is ferroelectric in the interval between the Curie temperatures 297 K and 255 K.

**Table 12.8** Refractivities for  $\lambda_0 \approx 589 \text{ nm}$ .

	$n_1 = n_2$	$n_3$
Diamond	2.4190(1)	
Silicon	4.21(2)	
LiF	1.3915(1)	
NaCl	1.5443(1)	
$\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	1.4564(1)	
$\text{CaF}_2$	1.43385(5)	
$\text{MgAl}_2\text{O}_4$	1.7274(1)	
$\text{Y}_3\text{Al}_5\text{O}_{12}$ (YAG)	1.823(1)	
$\alpha$ -Quartz (32)	1.54426(3)	1.55337(3)
Calcite $\text{CaCO}_3$ ( $\bar{3}m$ )	1.65835(5)	1.48640(5)
$\text{NaNO}_3$ ( $\bar{3}m$ )	1.5848(2)	1.3360(2)
Air (dry)	$n = 1.000272(2); dn/dT = -0.93(2) \cdot 10^{-6} \text{ K}^{-1}$	

**Table 12.9** Specific optic rotation for  $\lambda_0 = 589 \text{ nm}$ .

	$\alpha$ [grad $\text{mm}^{-1}$ ]
$\text{NaBrO}_3$ (23)	2.12
$\text{Na}_3\text{SbS}_4 \cdot 9\text{H}_2\text{O}$ (23)	2.35
$\alpha$ -Quartz (32)	21.72
Benzil $\text{C}_6\text{H}_5\text{CO} \cdot \text{COC}_6\text{H}_5$ (32)	24.84
$\text{LiIO}_3$ (6)	99.3
$\text{Al}(\text{IO}_3)_3 \cdot 2\text{HIO}_3 \cdot 6\text{H}_2\text{O}$ (6)	34.9

**Table 12.10** Coefficients of thermal expansion.

	$\alpha_{11}$ [ $10^{-6}\text{K}^{-1}$ ]	
Diamond	0.87	
Si	3.08(5)	
Cu	16.9(2)	
LiF	32.0(3)	
NaCl	39.1(3)	
KAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	13.6(2)	
CsAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	27.3(3)	
CaF <sub>2</sub>	19(1)	
$\alpha$ -Quartz (32)	13.3(3)	$\alpha_{33} = 7.07(7)$
Calcite ( $\bar{3}m$ )	-3.7(1)	$\alpha_{33} = 24.7(3)$
NaNO <sub>3</sub> ( $\bar{3}m$ )	8.8(3)	$\alpha_{33} = 107(3)$
Ca(HCOO) <sub>2</sub> (mmm)	-16.5(5)	$\alpha_{22} = 68.6(5)$ $\alpha_{33} = 29.8(5)$
Quartz glass (Spectrosil, $\rho = 2.200$ )	0.5(1)	

**Table 12.11** Magnetic susceptibilities in SI units.

	$\kappa_{11}$ [ $10^{-6}$ ]	$\kappa_{33}$
Diamond	-21.6	
Si	-3.3	
LiF	-12.9	
NaCl	-14.0	
CaF <sub>2</sub>	-14.3	
KAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	-11.7	
KCr(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	+280	
NH <sub>4</sub> Al(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	-11.1	
NH <sub>4</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	+650	
$\alpha$ -Quartz (32)	-15.6	-15.3
Calcite ( $\bar{3}m$ )	-12.1	-13.5

**Table 12.12** Coefficients of electric conductivities (a definitive indication of errors is not possible because of the large contributions from crystal defects).

	$s_{11}$ [ $\Omega^{-1}\text{cm}^{-1}$ ]	$s_{33}$
Al	$4 \cdot 10^5$	
Fe	$1.16 \cdot 10^5$	
Cu	$6.45 \cdot 10^5$	
Si (high-purity)	$5 \cdot 10^{-2}$	
NaCl	$2 \cdot 10^{-8}$	
Zn (6/mm)	$1.72 \cdot 10^5$	$1.62 \cdot 10^5$
LiIO <sub>3</sub> (50 Hz) (6)	$10^{-9}$	$0.5 \cdot 10^{-6}$
Bi ( $\bar{3}m$ )	$0.917 \cdot 10^4$	$0.725 \cdot 10^4$

**Table 12.13** Coefficients of thermal conductivity.

	$\lambda_{11}$ [ $\text{Jm}^{-1}\text{s}^{-1}\text{K}^{-1}$ ]		
Diamond (type I)	900(50)		
NaCl	6.2(2)		
$\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	0.605(6)		
$\text{CsAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	0.677(6)		
$\text{KH}_2\text{PO}_4$ (42)	$\lambda_{11} = 1.78(5)$	$\lambda_{33} = 1.36(4)$	
$\alpha$ -Quartz (32)	$\lambda_{11} = 6.2(3)$	$\lambda_{33} = 10.4(5)$	
$\text{NaNO}_3$ (3m)	$\lambda_{11} = 1.64(3)$	$\lambda_{33} = 2.14(7)$	
$\text{Ca}(\text{HCOO})_2$ (mmm)	$\lambda_{11} = 1.35(2)$	$\lambda_{22} = 0.561(5)$	$\lambda_{33} = 0.99(1)$

**Table 12.14** Adiabatic piezoelectric constants for low frequencies (about 10 kHz).

	$d_{ijk}$ [ $\text{pCn}^{-1}$ ] ( $= [10^{-12}\text{mV}^{-1}]$ )		
$\text{NaBrO}_3$ (23)	$d_{123} = 1.21(1)$		
$\text{KH}_2\text{PO}_4$ (42)	$d_{123} = 0.65(2),$	$d_{312} = -10.5(2)$	
$\alpha$ -Quartz (32)	$d_{111} = 2.31(1),$	$d_{123} = -0.37(1)$	
$\text{LiNbO}_3$ (3m)	$d_{113} = 37.0(3),$	$d_{222} = 20.8(1)$	$d_{311} = -0.86(2)$
	$d_{333} = 16.2(2)$		

**Table 12.15** Adiabatic electrooptic constants for low frequencies (about 10 kHz) and  $\lambda = 633$  nm (except for GaAs).

	$r_{ijk}$ [ $\text{pm V}^{-1}$ ]		
$\text{NaBrO}_3$ (23)	$r_{123} = 0.57(3)$		
$\text{NaClO}_3$ (23)	$r_{123} = 0.40(2)$		
GaAs (43)	$r_{123} = 1.43(7)$ (1150 nm)		
Hexamethylenetetramine (43)	$r_{123} = 0.80(5)$		
$\text{KH}_2\text{PO}_4$ (42)	$r_{123} = 10.3(2)$	$r_{231} = 8.6(2)$	
$\alpha$ -Quartz (32)	$r_{111} = 0.48(1)$	$r_{231} = 0.23(1)$	
$\text{LiNbO}_3$ (3m)	$r_{113} = 9.6$	$r_{222} = 6.8$	
	$r_{311} = 32.6$	$r_{333} = 30.9$	

**Table 12.16** Nonlinear optical coefficients  $\epsilon_{ijk}^* = \epsilon_0^{-1}\epsilon_{ijk}$  for the vacuum wavelength of the primary wave  $\lambda = 1064$  nm (Nd glass laser).

	$\epsilon_{ijk}^*$ [ $10^{-12}\text{V}^{-1}\text{m}$ ]		
GaAs (43)	$\epsilon_{123}^* = 134$		
$\text{LiIO}_3$ (6)	$\epsilon_{311}^* = -7.1;$	$\epsilon_{333}^* = -7.0;$	$\epsilon_{123}^* = 0.31$
$\text{KH}_2\text{PO}_4$ (42)	$\epsilon_{312}^* = 0.63$		
$\text{NH}_4\text{H}_2\text{PO}_4$ (42)	$\epsilon_{312}^* = 0.76$		
$\text{LiNbO}_3$ (3m)	$\epsilon_{311}^* = 5.9;$	$\epsilon_{333}^* = -34;$	$\epsilon_{222}^* = 4.0$
$\alpha$ -Quartz (32)	$\epsilon_{111}^* = 0.50;$	$\epsilon_{123}^* = -0.005$	
$\alpha$ -HIO <sub>3</sub> (22)	$\epsilon_{123}^* = 8.3$		

**Table 12.17** Elastic constants  $c_{ij}$  [ $10^{10}\text{N m}^{-2}$ ].

	$c_{11}$	$c_{12}$	$c_{44} = c_{66}$
Diamond	104	17	55
Si	16.5(1)	6.4(1)	7.92(3)
LiF	11.37(2)	4.76(3)	6.35(3)
NaCl	4.944(8)	1.29(2)	1.266(5)
$\gamma$ -NaCN	2.534(2)	1.444(6)	0.033(1)
CsCl	3.64(1)	0.92(2)	0.80(1)
CaF <sub>2</sub>	16.357(20)	4.401(16)	3.392(13)
Y <sub>3</sub> Ga <sub>5</sub> O <sub>12</sub>	28.70(1)	11.60(6)	9.04(4)
KAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	2.465(3)	1.021(8)	0.867(5)
CsAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	3.118(5)	1.541(9)	0.840(5)
NaBrO <sub>3</sub>	5.478(5)	1.628(6)	1.505(5)
KH <sub>2</sub> PO <sub>4</sub> ( $\bar{4}2$ )	$c_{11} = 7.165(5)$ $c_{13} = 1.494(8)$	$c_{33} = 5.640(5)$ $c_{66} = 0.621(4)$	$c_{12} = -0.627(6)$ $c_{44} = 1.248(6)$
$\alpha$ -Quartz (32)	$c_{11}^E = 8.674$ $c_{13}^E = 1.19$	$c_{33}^E = 10.72$ $c_{44}^E = 5.79$	$c_{12}^E = 0.698$ $c_{14}^E = -1.79$
Ga (mmm)	$c_{11} = 10.16(1)$ $c_{12} = 4.601(10)$ $c_{66} = 4.079(10)$	$c_{22} = 9.156(10)$ $c_{13} = -3.057(10)$ $c_{55} = 4.155(10)$	$c_{33} = 13.64(1)$ $c_{23} = 2.804(10)$ $c_{44} = 3.499(10)$

**Table 12.18** Thermoelastic constants  $T_{ij} = d \log c_{ij} / dT$  [ $10^{-3}\text{K}^{-1}$ ].

	$T_{11}$	$T_{12}$	$T_{44} = T_{66}$
Diamond	-0.0137	-0.057	-0.0125
Si	-0.081	-0.11	-0.063
LiF	-0.66	+0.01	-0.28
NaCl	-0.80	+0.17	-0.266
$\gamma$ -NaCN	+0.47	-1.38	+27
CsCl	-0.42	-0.93	-1.29
CaF <sub>2</sub>	-0.205	-0.291	-0.343
Y <sub>3</sub> Ga <sub>5</sub> O <sub>12</sub>	-0.113	-0.092	-0.092
KAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	+0.108	+1.91	-0.95
CsAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	-0.517	-0.69	-0.43
NaBrO <sub>3</sub>	-0.72	-0.45	-0.58
KH <sub>2</sub> PO <sub>4</sub> ( $\bar{4}2$ )	$T_{11} = -0.635$ $T_{13} = -0.185$	$T_{33} = -0.49$ $T_{66} = -0.53$	$T_{12} = -0.62$ $T_{44} = -0.57$
$\alpha$ -Quartz (32)	$T_{11} = -0.0443$ $T_{13} = -0.55$	$T_{33} = -0.160$ $T_{44} = -0.175$	$T_{12} = -2.69$ $T_{14} = +0.11$
Ga (mmm)	$T_{11} = -0.47$ $T_{12} = -0.029$ $T_{66} = -0.72$	$T_{22} = -0.42$ $T_{13} = +0.05$ $T_{55} = -0.43$	$T_{33} = -0.38$ $T_{23} = +0.115$ $T_{44} = -0.59$

**Table 12.19** Piezoelastic constants  $P_{ij} = dc_{ij}/dp$  (dimensionless).

	$P_{11}$	$P_{12}$	$P_{44}$	$\frac{dK^{-1}}{dp}$
Diamond	5.72	4.18	3.19	4.69
Si	4.32	4.22	0.80	4.26
LiF	9.86	2.76	1.40	5.12
NaCl	11.85	2.06	0.37	5.32
$\gamma$ -NaCN	5.55	5.98	-0.36	5.84
CsCl	6.77	5.13	3.52	5.68
CaF <sub>2</sub>	6.11	4.55	1.32	5.07
KAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	6.73	7.15	2.77	7.01
CsAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	5.83	6.05	1.17	5.98
MgAl <sub>2</sub> O <sub>4</sub>	5.08	4.93	0.86	4.98
K <sub>2</sub> Hg(CN) <sub>4</sub>	-6.51	-6.23	-1.22	-6.32
$\alpha$ -Quartz (32)	$P_{11} = 3.30$ $P_{13} = 5.95$	$P_{33} = 10.93$ $P_{44} = 2.66$	$P_{12} = 83.7$ $P_{14} = 2$	$\frac{dK^{-1}}{dp} = 19.8$

**Table 12.20** Piezooptic constants  $q_{ij}$  [ $10^{-12}\text{m}^2\text{N}^{-1}$ ] and elasto-optic constants  $p_{ij}$  (dimensionless) for  $\lambda_0 = 589\text{ nm}$ . Abbreviations:  $q_{11} = q_{1111}$ ;  $q_{12} = q_{1122}$ ;  $q_{44} = 2q_{2323}$  etc.;  $p_{11} = p_{1111}$ ;  $p_{12} = p_{1122}$ ;  $p_{44} = p_{2323}$  etc.

	$q_{11}$	$q_{12}$	$q_{44}$	$p_{11}$	$p_{12}$	$p_{44}$
LiF (4/m3)	-0.40	1.12	-0.83	0.061	0.161	-0.053
NaCl (4/m3)	1.27	2.58	-0.84	0.129	0.177	-0.011
RbI (4/m3)	9.23	4.99	-7.92	0.275	0.181	-0.022
CaF <sub>2</sub> (4/m3)	-0.33	1.10	0.74	0.038	0.226	0.0254
Hexamethylenetetramine ( $\bar{4}3$ )	11.95	8.42	7.56	0.259	0.227	0.039
KAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O (m3)	2.43	6.66	-0.55	0.199	0.260	-0.005
CsAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O (m3)	$q_{13} = 6.99$			$p_{13} = 0.265$		
	-0.63	4.25	-1.82	0.124	0.201	-0.015
$\alpha$ -Quartz (32)	$q_{13} = 5.05$			$p_{13} = 0.214$		
	$q_{11} = 1.25$			$p_{11} = 0.15$		
	$q_{12} = 2.60$			$p_{12} = 0.26$		
	$q_{13} = 1.95$			$p_{13} = 0.265$		
	$q_{14} = -0.10$			$p_{14} = -0.029$		
	$q_{31} = 2.94$			$p_{31} = 0.27$		
	$q_{33} = 0.12$			$p_{33} = 0.10$		
	$q_{41} = -0.33$			$p_{41} = -0.045$		
	$q_{44} = -1.07$			$p_{44} = -0.074$		

**Table 12.21** Nonlinear elastic coefficients  $c_{ijk}$  [ $10^{10}\text{N m}^{-2}$ ]; definition according to Brugger (1964).

	$c_{111}$	$c_{112}$	$c_{113}$	$c_{123}$	$c_{144}$	$c_{155}$	$c_{166}$	$c_{456}$
Si (4/m3)	-81.5	-44.8	-44.8	-7.0	-31	-31	-31	-7.5
LiF (4/m3)	-142	-26.4	-26.4	15.6	8.5	-27.3	-27.3	9.4
NaCl (4/m3)	-84.3	-3.3	-3.3	-3.6	2.0	-6.0	-6.0	2.0
CaF <sub>2</sub> (4/m3)	-124.6	-40	-40	-25.4	-12.4	-21.4	-21.4	-7.5
KAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O (m3)	-22.2	-7.1	-8.6	-13.4	-2.3	-8.0	-7.44	-2.0
CsAl(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O (m3)	-21.2	-11.1	-12.6	-9.0	-2.7	-5.90	-5.36	-1.6
$\alpha$ -Quartz (32)	$c_{111} = -21.4;$ $c_{123} = 28.2;$ $c_{144} = -15.8;$ $c_{344} = -12.9;$	$c_{112} = -34.1;$ $c_{124} = -2.0;$ $c_{155} = -17.9;$ $c_{444} = -22.6;$	$c_{113} = +1.9;$ $c_{133} = -31.8;$ $c_{222} = -33.6;$	$c_{114} = -15.5;$ $c_{134} = +35;$ $c_{333} = -82.6;$				

## 12.6

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## 12.6.1

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- Vol. III/16a,b : Ferroelectrics and related substances (1981, 1982).
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- Vol. III/18a,b : Ferroelectrics and related substances (1990).
- Vol. III/29a : Low frequency properties of dielectric crystals: Second and higher order elastic constants (1992).
- Vol. III/29b : Low frequency properties of dielectric crystals: Piezoelectric, pyroelectric and related constants (1993).
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## 12.6.4

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Acta Crystallographica

Crystal Research and Technology

Journal of Applied Crystallography

Journal of Crystal Growth

Kristallografiya (Soviet Physics Crystallography)

physica status solidi

Solid State Communications

Zeitschrift für Kristallographie

In addition, almost all Journals in physics and physical chemistry contain articles on crystal physics.