

# I Introduction

## IA General remarks

The present Volume III/36, which consists of three Subvolumes A, B and C, is a revised, updated and extended edition of Landolt-Börnstein, New Series, Group III, Vol. 16 "Ferroelectrics and Related Substances" [81Mit, 82Mit] and Vol. 28 (supplement to Vol. 16) [90Nak1, 90Nak2]. In the compilation work for the last volume III/28, survey was made mainly on the references published before 1986. Since then many papers were published concerning ferroelectricity, as indicated by that the Toyoda bibliography [93Toy] contains about 30 000 papers published on ferroelectrics between 1987 and 1993. During this period and the succeeding years, many ferroelectrics were discovered and new experimental techniques were developed. This new edition III/36 is planned in response to this situation.

Materials treated in Vol. III/36 are ferroelectric and antiferroelectric substances (including solid solutions) as well as substances closely related to them. The Subvolume A is for oxides, B for inorganic substances other than oxides, and C for organic crystals, liquid crystals and polymers. The data included in Vol. III/36 are those which give information on the ferroelectric or antiferroelectric character of the substance and are important in connection with it. Figures and tables are presented only when they seemed to be reliable. In some cases, references are given without presenting numerical data for user's convenience. The compilation of data has been made on the basis of a bibliography prepared by Toyoda [93Toy] and a supplement to it, covering the years from 1920, when Valasek found the ferroelectric effect in Rochelle salt, till the end of 1995. INSPEC also was helpful to search data. More recent data, published in 1996, have been taken into account as far as possible. The bibliography [93Toy] includes 71 300 references to literature on ferroelectrics and related substances from 1920 to 1993. The number of ferroelectrics families increases from 48 in III/28 to 72 in III/36. The numbers of tables and figures increase from 727 and 3277 in III/16b and III/28b (supplement to III/16b) to 949 and 3553 in III/36B, respectively. The article [05Mit] will be helpful to survey all the contents of III/36.

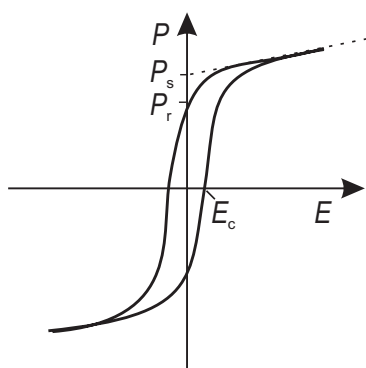
It should be noted that the number assigned to the same material is different in different ferroelectrics LB volumes (III/3, III/9, III/16, III/28 and III/36), since the numbering was made in the order of simplicity of chemical formula including ferroelectrics found at each stage.

## Printed version and electronic version on CD-ROM

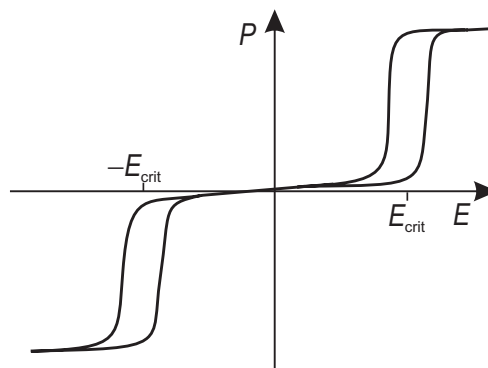
This subvolume consists of a printed version and an electronic version on CD-ROM. All the compiled data can be found on the CD-ROM. Abundance and diversity of the data, however, makes it difficult to overview the relevant research field, and thus the printed version is designed to survey the present status of ferroelectrics research and to grasp the contents of the CD-ROM. About 8 % of the tables and 31 % of the figures on the CD-ROM are selected and presented in the printed version. Captions of the tables and figures which appear only on the CD-ROM are presented also in the printed version.

## IB Definition of ferroelectrics and antiferroelectrics

A ferroelectric crystal is defined as a crystal which belongs to the pyroelectric family (i.e. shows a spontaneous electric polarization), and whose direction of spontaneous polarization can be reversed by an electric field. An antiferroelectric crystal is defined as a crystal whose structure can be considered as being composed of two sublattices polarizing spontaneously in antiparallel directions at least in one projection, and whose ferroelectric phase can be induced by applying an electric field. Experimentally the reversal of the spontaneous polarization in ferroelectrics is observed as a single hysteresis loop (Fig. IB-1), and the induced phase transition in antiferroelectrics as a double hysteresis loop (Fig. IB-2), when a low-frequency ac field of a suitable strength is applied.



**Fig. IB-1.** Ferroelectric hysteresis loop.  $P_s$ : spontaneous polarization (see remarks on  $P_s$  in IC).  $P_r$ : remanent polarization.  $E_c$ : coercive field.



**Fig. IB-2.** Antiferroelectric hysteresis loop.  $E_{crit}$ : critical field.

The spontaneous polarization in ferroelectrics and the sublattice polarizations in antiferroelectrics are analogous to their magnetic counterparts. As described above, however, these polarizations are a necessary, but not a sufficient condition for ferroelectricity or antiferroelectricity. In other words, ferroelectricity and antiferroelectricity are concepts based not only upon crystal structure, but also upon the dielectric behavior of the crystal. It is a common dielectric character of ferroelectrics and antiferroelectrics that in a certain temperature range the dielectric polarization is observed as a two-valued function of the electric field strength as shown in Figs. IB-1 and IB-2.

In general, the spontaneous polarization in ferroelectrics or the sublattice polarization in antiferroelectrics can be regarded as a structural perturbation on a nonpolarized crystal. Such a non-perturbed crystal structure is sometimes called a paraelectric structure. By definition, the paraelectric structure can be realized by making the ferroelectric polarization or the sublattice polarization equal to zero. The phase having a paraelectric structure is called a paraelectric phase. Usually ferroelectrics or antiferroelectrics exhibit the paraelectric phase at high temperatures.

Some structural perturbation on a paraelectric state results in a state which neither has a spontaneous polarization nor fits in the definition of antiferroelectrics. Such a crystal state is called nonpolar in this volume.

## Ferroelectricity in liquid crystals and polymers

In the last three decades active studies have been made on ferroelectric liquid crystals and polymers, after ferroelectricity had been considered as a characteristic property of solid crystals or ceramics for about 50 years. Ferroelectricity of these non-solid materials is attractive because of their applications to fast display elements and soft transducers, in addition to the pure scientific interest.

Ferroelectric liquid crystals are defined as those which exhibit the ferroelectric hysteresis loop as shown in Fig. IB-1. Unlike the ferroelectric crystals, however, these ferroelectric liquid crystals have no spontaneous polarization as a bulk in general. For instance, the chiral smectic C phase of DOBAMBC consists of many layers, each of which has spontaneous polarization parallel to the layer plane, but the spontaneous polarization is helically distributed in different directions from layer to layer, so that the bulk of DOBAMBC has no spontaneous polarization as a whole. Although this structural feature is somewhat similar to antiferroelectrics, the observed hysteresis loop becomes the one as shown in Fig. IB-1 because the helical structure does not have a chance to appear under the alternating electric field due to its transition delay and direct reversal of the polarization occurs between the induced ferroelectric phases, and thus the linear part of the antiferroelectric hysteresis in Fig. IB-2 is eliminated. Some liquid crystals exhibit the antiferroelectric hysteresis loop as shown in Fig. IB-2 when the linear part appears and are called antiferroelectric. Data on ferroelectric, antiferroelectric and related liquid crystals are given in Chap. 71. Readers may consult [91Goo], [91Tay], [93Buk], [94Bli], [94Fuk], [98Bli] for ferroelectric

and antiferroelectric liquid crystals, and [80deJ], [92Cha], [93deG], [97Col] for a general review on liquid crystals.

Ferroelectric polymers are usually prepared as thin films in which crystalline and amorphous regions coexist, and the ferroelectric hysteresis loop originates from reversal of spontaneous polarization in the crystal region [89Fur]. The electric field distribution is expected to be complex in the thin film because of the interposition of the amorphous region. The ferroelectric hysteresis loop can be observed when the volume ratio of the crystal regions per total is relatively large (e.g., more than 50 %). The coercive field is larger (e.g., > 50 MV/m) compared to that of the solid ferroelectrics (usually a few MV/m or smaller). Ferroelectric properties sensitively depend upon sample preparation, e.g., melt-quenching, melt-extrusion, annealing temperature, poling, etc. [89Fur] and [97Kod]. Data on polymer ferroelectrics are presented in Chap. 72.

## IC Remarks on some fundamental concepts and quantities

### Data at room temperature

Throughout this volume, data in tables and figures should be understood as room temperature data if not otherwise stated.

### Presentation of experimental errors

In the tables of this volume, experimental errors are given in parentheses referring to the last decimal places. For example, 1.356(12) stands for  $1.356 \pm 0.012$  and 127.3(21) for  $127.3 \pm 2.1$ .

### Chemical formulae

For all the complex perovskite-type oxides, chemical formulae such as  $\text{Pb}(\text{Fe}_{1/2}\text{Nb}_{1/2})\text{O}_3$  or  $\text{Pb}(\text{Fe}_{2/3}\text{W}_{1/3})\text{O}_3$  are used instead of formulae such as  $\text{Pb}_2(\text{FeNb})\text{O}_6$  or  $\text{Pb}_3(\text{Fe}_2\text{W})\text{O}_9$  even when the oxides have the ordered structure.

### Molecular weight

The molecular weight  $M$  is given following the chemical formula at the beginning of each section. It was calculated with the atomic weight (the ratio of the mass per mole of the elements to 1/12 of the mass of one mole of nuclides  $^{12}\text{C}$ ) recommended by the Commission on Atomic Weights and Isotopic Abundances of IUPAC in 1985 [86IUP].

The following remarks are made according to the order of the subsections of Table IF-1. The number in parentheses corresponds to that of the relevant subsection.

### History of research (1)

Brief description is made on the history of research of the substance in each subsection 1a. In Section ID, Figs. ID-1...3 give a survey on the history of research of ferroelectrics.

### Name of phase and symbols for space group (1)

Phases are numbered as I, II, ... beginning with the high temperature phase. Space group is given both by the international symbol and the Schoenflies symbol (e.g.  $\text{P2}_1\text{-C}_2^2$ ). See [92Wil], for symbols of the 4-dimensional superspace groups for incommensurate phases.

### Diffuse phase transitions (1)

The ferroelectric phase transition takes place in a relatively wide temperature range in disordered perovskite-type oxides of complex compositions [e.g.  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ ], and in some solid solutions of tungsten-bronze-type oxides, etc. It is called a diffuse (or smeared) phase transition. In such cases the transition temperature  $\Theta_f$  can be given only as an average value, and is presented with (average), [e.g.

140 °C (average)] in figures and tables of this volume. Usually the average value of  $\Theta$  is determined as the peak position in the curve of low-frequency dielectric constant vs. temperature.

### Crystal structure (3)

Most crystallographic nomenclatures are the same as in the International Tables for Crystallography [65Lon], [83Hah], [92Wil]. Data expressed in kX units have been transformed to Å units according to the conversion factor 1 kX = 1.00202 Å [48Bra]. For some crystals, different systems of crystallographic  $a$ ,  $b$ ,  $c$  axes are used in literature. The  $a$ ,  $b$ ,  $c$  axes adopted in this volume are those which seem to be most widely used.

The notation  $[uvw]$  should be understood as a direction referred to the  $a$ ,  $b$ ,  $c$  axes in the paraelectric phase unless otherwise stated. The  $X$ ,  $Y$ ,  $Z$  axes (the rectangular coordinates to describe vector and tensor quantities) are parallel to the  $a$ ,  $b$ ,  $c$  axes, respectively, when the  $a$ ,  $b$ ,  $c$  axes are perpendicular to each other. In the monoclinic system (taking  $b$  parallel to the unique axis)  $Y \parallel b$ ,  $Z \parallel c$ , and  $X$  forms a right-handed rectangular system along with the  $Y$  and  $Z$  axes.

In crystal structure analysis, the atomic scattering factor is corrected for the thermal vibration by the temperature factor. Various expressions have been proposed for it. The most frequently used ones are as follows.

Temperature factor

$$= \exp\{-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{23}kl + B_{31}lh)\} \quad (a)$$

$$= \exp\{-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + 2b_{12}hk + 2b_{23}kl + 2b_{31}lh)\} \quad (b)$$

$$= \exp\{-1/4 (a^{*2}\beta_{11}h^2 + b^{*2}\beta_{22}k^2 + c^{*2}\beta_{33}l^2 + 2a^*b^*\beta_{12}hk + 2b^*c^*\beta_{23}kl + 2c^*a^*\beta_{31}lh)\} \quad (c)$$

$$= \exp\{-2\pi^2 (a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2b^*c^*U_{23}kl + 2c^*a^*U_{31}lh)\} \quad (d)$$

where  $B_{ij}$ ,  $b_{ij}$ ,  $\beta_{ij}$ , and  $U_{ij}$  are called temperature parameters. Sometimes the factor is approximately expressed as:

$$\text{Temperature factor} = \exp(-B \sin^2 \theta / \lambda^2), \quad (e)$$

where  $B$  is called isotropic temperature parameter or Debye parameter. In a few publications the mean square displacement of the atom,  $\overline{u^2} = B/(8\pi^2)$ , is listed instead of  $B$ .

### Discrepancy indices in structure analysis (3)

As a measure of reliability of the result of structure analysis of a crystal, the discrepancy index  $R$  (sometimes called reliability factor) is used, which is defined by

$$R = \sum | |F_i^{\text{obs}}| - |F_i^{\text{calc}}| | / \sum |F_i^{\text{obs}}|,$$

where  $F_i$  is the structure factor of the  $i^{\text{th}}$  Bragg reflection, and the summation is extended over all the observable  $F_i$ 's.

In powder diffraction studies, the discrepancy index  $R_B$  of intensity is used, which is defined by

$$R_B = \sum |I_i^{\text{obs}} - I_i^{\text{calc}}| / \sum I_i^{\text{obs}},$$

where  $I_i$  is the integrated intensity of the  $i^{\text{th}}$  Bragg peak. In powder diffraction studies, the profile of the diffraction peak is another source of information on the crystal structure. Structure analysis taking the peak profile into account is usually called Rietveld profile refinement method due to his original work [67Rie]. In this method, all the crystallographic parameters (i.e. atomic positions, temperature parameters and the unit cell parameters) are refined simultaneously on the basis of a least square fitting procedure. As a measure of fitness to experimental data, the following discrepancy index  $R_{\text{prof}}$  is used

$$R_{\text{prof}} = \frac{w_i \left( y_i^{\text{obs}} - s y_i^{\text{calc}} \right)^2}{w_i \left( y_i^{\text{obs}} \right)^2}^{\frac{1}{2}},$$

where  $y_i$  is the intensity of scattered X-rays (or neutrons) at the scattering angle  $2\theta_i$ , and  $s$  is the scale factor (also adjusted during the refinement), and  $w_i$  is the weight given by intensity statistics (e.g.  $w_i = 1/y_i^{\text{obs}}$ ).

In the case of neutron diffraction studies,  $R_{\text{nuc}}$  and  $R_{\text{magn}}$  are defined as discrepancy indices for nuclear and magnetic scatterings, respectively.

### Dielectric and electrocaloric properties (5)

For methods of measuring dielectric constants at various frequencies readers may consult Field and Westphal's article in [54von]. The isothermal dielectric permittivity  $\epsilon_{ij}$  and pyroelectric (or electrocaloric) coefficient  $p_i$  are defined by the equations:

$$\Delta D_i = \sum_j \epsilon_{ij} E_j + p_i \Delta T,$$

$$\Delta S = \sum_j p_j E_j + (\rho c_p / T) \Delta T,$$

where  $\Delta D_i$ ,  $\Delta T$ , and  $\Delta S$  are changes of the component of electric displacement, temperature and entropy, respectively, and  $E_j$ ,  $\rho$ ,  $c_p$  and  $T$  are the component of electric field strength, density, specific heat capacity and the absolute temperature, respectively. With  $\Delta S = 0$  in the above equations we have the expression for the adiabatic dielectric permittivity  $\epsilon_{ij}^S$ :

$$\epsilon_{ij}^S = \epsilon_{ij} - (T/\rho c_p) p_i p_j.$$

The dielectric permittivities measured with the alternating current should be regarded as  $\epsilon_{ij}^S$ .

Nonlinear properties of the polarization  $\mathbf{P}$  and the strain  $\mathbf{S}$  against the electric field  $\mathbf{E}$  and the stress  $\mathbf{T}$  are characteristic of ferro- and antiferroelectrics. At constant temperature and stress, the electric field strength  $E$  is expressed by the Taylor series expansion as

$$E = (1/\chi_p)P + \xi P^3 + \zeta P^5.$$

Therefore, values of  $\xi$  and  $\zeta$  are given as measures of the dielectric nonlinearity. They should be understood as the values at atmospheric pressure unless otherwise stated. Values of  $\chi_p$  are not given in this volume, but, in the paraelectric phase, they can be calculated with the relation

$$\chi_p = \epsilon_0(\kappa - 1),$$

where  $\kappa$  is the dielectric constant. In general,  $\kappa$  obeys the Curie-Weiss law above the Curie point:

$$\kappa = \kappa_\infty + C/(T - \Theta_p),$$

where  $\kappa_\infty$  is a temperature-independent term and sometimes small enough to be neglected compared with the term  $C/(T - \Theta_p)$ .

Usually the spontaneous polarization  $P_s$  is determined by the extrapolation of the linear section of the hysteresis loop from high values of  $E$  to the  $P$  axis as shown in Fig. IB-1. But a few research workers determine  $P_s$  by putting it equal to the remanent polarization  $P_r$ . In general, however, the difference between  $P_s$  obtained by the extrapolation and  $P_r$  is within the experimental error.

### Electromechanical and elastic properties (7, 8)

Latin subscripts  $i$  and  $j$  stand for 1, 2, 3, and Greek subscripts  $\lambda$ ,  $\mu$ , and  $\nu$  for 1...6. The correspondence between  $i$ ,  $j$  and  $\lambda$  (or  $\mu$ ,  $\nu$ ) is as usual: 1, 1 $\leftrightarrow$ 1; 2, 2 $\leftrightarrow$ 2; 3, 3 $\leftrightarrow$ 3; 2, 3 $\leftrightarrow$ 4; 3, 1 $\leftrightarrow$ 5; 1, 2 $\leftrightarrow$ 6.

In this volume the sign of the component  $T_{ij}$  of the stress tensor is defined as positive when it produces a positive strain  $S_{ij}$ . The strain component is related to the component  $S_{ij}$  of the strain tensor by

$$\begin{aligned} S_\lambda &= S_{ij} \quad \text{for } i = j, \\ S_\lambda &= 2S_{ij} \quad \text{for } i \neq j. \end{aligned}$$

Taking the electrostriction into account,  $S$  is given by

$$S_\lambda = \sum_{\mu} s_{\lambda\mu}^p T_\mu + \sum_i f_{i\lambda} P_i + \sum_{ij} Q_{\lambda ij} P_i P_j.$$

The electrostrictive constants  $Q_{\lambda\mu}$  are defined by

$$\begin{aligned} Q_{\lambda\mu} &= Q_{\lambda ij} \quad \text{for } i = j, \\ Q_{\lambda\mu} &= 2Q_{\lambda ij} \quad \text{for } i \neq j. \end{aligned}$$

Other constants related to electromechanical and elastic properties are defined in the same manner and expressed by the same symbols as in 2.1 of [66Bec]. Relations associated with electromechanical and elastic constants are summarized in Table IC-1. Definitions and symbols of quantities related to electrooptic and piezooptic effects are the same as in 3.1 of [66Bec]. Relations associated with electrooptic and piezooptic constants are summarized in Table IC-2. For detailed discussions on interaction between vector and tensor quantities readers are referred to [57Nye] and [66Mas]. Readers may consult [86Lan] for theory of elasticity. For general reviews on electromechanical properties readers may consult [46Cad], [50Mas], [64Mas], [93Bha] and [96Coo]. For second and higher order elastic constants, see [92Eve]. For piezoelectric ceramics, see [71Jaf].

**Table IC-1. Electromechanical and elastic constants: relations and definitions**

#### (1) Piezoelectric equations

$$\begin{aligned} D_i &= \sum_j \epsilon_{ij}^T E_j + \sum_{\mu} d_{i\mu} T_\mu & E_i &= \sum_j \beta_{ij}^T D_j - \sum_{\mu} g_{i\mu} T_\mu \\ S_\lambda &= \sum_j d_{j\lambda} E_j + \sum_{\mu} s_{\lambda\mu}^E T_\mu & S_\lambda &= \sum_j g_{j\lambda} D_j + \sum_{\mu} s_{\lambda\mu}^D T_\mu \\ D_i &= \sum_j \epsilon_{ij}^S E_j + \sum_{\mu} e_{i\mu} S_\mu & E_i &= \sum_j \beta_{ij}^S D_j + \sum_{\mu} h_{i\mu} S_\mu \\ T_\lambda &= - \sum_j e_{j\lambda} E_j + \sum_{\mu} c_{\lambda\mu}^E S_\mu & T_\lambda &= - \sum_j h_{j\lambda} D_j + \sum_{\mu} c_{\lambda\mu}^D S_\mu \end{aligned}$$

#### (2) Relations between various constants

$$\begin{aligned} \sum_{\nu} s_{\lambda\nu}^+ c_{\mu\nu}^+ &= \delta_{\lambda\mu} \quad (+ = E \text{ or } D) & \sum \beta_{ik}^* \epsilon_{ik}^* &= \delta_{ij} \quad (* = \mathbf{S} \text{ or } \mathbf{T}) \\ e_{i\lambda} &= \sum_{\mu} d_{i\mu} c_{\mu\lambda}^E & d_{i\lambda} &= \sum_{\mu} e_{i\mu} s_{\mu\lambda}^E \\ h_{i\lambda} &= \sum_{\mu} g_{i\mu} c_{\mu\lambda}^D & g_{i\lambda} &= \sum_{\mu} h_{i\mu} s_{\mu\lambda}^D \\ e_{i\lambda} &= \sum_{ij} \epsilon_{ij}^S h_{j\lambda} & d_{i\lambda} &= \sum_{ij} \epsilon_{ij}^T g_{j\mu} \end{aligned}$$

$$\begin{aligned}
 h_{i\lambda} &= \sum \beta_{ij}^{\mathbf{S}} e_{j\lambda} & g_{i\lambda} &= \sum \beta_{ij}^{\mathbf{T}} d_{j\lambda} \\
 c_{\lambda\mu}^{\mathbf{D}} - c_{\lambda\mu}^{\mathbf{E}} &= \sum h_{j\lambda} e_{j\mu} & s_{\lambda\mu}^{\mathbf{D}} - s_{\lambda\mu}^{\mathbf{E}} &= - \sum g_{j\lambda} d_{j\mu} \\
 \beta_{ij}^{\mathbf{S}} - \beta_{ij}^{\mathbf{T}} &= \sum h_{i\mu} g_{j\mu} = \sum h_{j\mu} g_{i\mu} & \epsilon_{ij}^{\mathbf{S}} - \epsilon_{ij}^{\mathbf{T}} &= - \sum e_{i\mu} d_{j\mu} = - \sum e_{j\mu} d_{i\mu} \\
 \delta_{\lambda\mu} &= \begin{cases} 1 & \text{for } \lambda = \mu \\ 0 & \text{for } \lambda \neq \mu \end{cases} & \delta_{ij} &= \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases}
 \end{aligned}$$

(3) Definitions of various electromechanical coupling factors.

The coupling factor  $k_{i\lambda}$  is defined by  $k_{i\lambda}^2 = d_{i\lambda}^2 (\epsilon_{ii}^{\mathbf{T}} s_{\lambda\lambda}^{\mathbf{E}})^{-1}$ .

The following two coupling factors are used as well:

a) planar coupling factor

$$k_p^2 = \frac{2d_{31}^2}{\epsilon_{33}^{\mathbf{T}} (s_{11}^{\mathbf{E}} + s_{12}^{\mathbf{E}})} = \frac{2}{1 - \sigma^{\mathbf{E}}} k_{31}^2$$

for a thin disc of piezoelectric ceramics which is poled perpendicular to it ( $\sigma^{\mathbf{E}}$ : Poisson ratio).

b) thickness coupling factor  $k_t^2 = e_{33}^2 (\epsilon_{33}^{\mathbf{S}} c_{33}^{\mathbf{D}})^{-1}$  for a thin plate the thickness of which is along  $Z$ .

(4) Definitions of electrostrictive constants.

$$S_{\lambda} = \sum Q_{\lambda ij} P_i P_j \quad \text{and} \quad Q_{\lambda\mu} = \begin{cases} Q_{\lambda ij} & \text{for } i = j \\ 2Q_{\lambda ij} & \text{for } i \neq j \end{cases}$$

**Table IC-2. Electrooptic and piezoelectric constants: relations and definitions**

(1) Index ellipsoid

$$a_1 x^2 + a_2 y^2 + a_3 z^2 + 2a_4 yz + 2a_5 zx + 2a_6 xy = 1.$$

(2) Piezoelectric and electrooptic equations

$$\Delta a_{\lambda} = \sum \Pi_{\lambda\nu}^{\mathbf{E}} T_{\nu} + \sum r_{\lambda i}^{\mathbf{T}} E_i + \sum L_{\lambda ij}^{\mathbf{T}} E_i E_j, \quad \Delta a_{\lambda} = \sum p_{\lambda\nu}^{\mathbf{E}} S_{\nu} + \sum r_{\lambda i}^{\mathbf{S}} E_i + \sum L_{\lambda ij}^{\mathbf{S}} E_i E_j$$

$$\Delta a_{\lambda} = \sum \Pi_{\lambda\nu}^{\mathbf{P}} T_{\nu} + \sum \rho_{\lambda i}^{\mathbf{T}} P_i + \sum M_{\lambda ij}^{\mathbf{T}} P_i P_j, \quad \Delta a_{\lambda} = \sum p_{\lambda\nu}^{\mathbf{P}} S_{\nu} + \sum \rho_{\lambda i}^{\mathbf{S}} P_i + \sum M_{\lambda ij}^{\mathbf{S}} P_i P_j$$

and

$$L_{\lambda\mu}^* = \begin{cases} L_{\lambda ij}^* & \text{for } i = j \\ 2L_{\lambda ij}^* & \text{for } i \neq j \end{cases} \quad M_{\lambda\mu}^* = \begin{cases} M_{\lambda ij}^* & \text{for } i = j \\ 2M_{\lambda ij}^* & \text{for } i \neq j \end{cases} \quad (* = \mathbf{S} \text{ or } \mathbf{T})$$

### Acoustic surface waves (8)

The acoustic surface waves were treated first by Lord Rayleigh in 1885. They propagate through the thin surface region with smaller velocities than bulk elastic waves. Recently engineers have been interested in these properties of the surface waves for constructing signal-processing devices. Basic data on the surface waves are presented in subsection 8a. Readers may consult [70Whi], [70Far] and [78Oli] for basic properties of the surface waves and recent development in application, and refer to [68Cam] and [72Far] for analytic treatment of various devices.

### Optical properties (9)

For general reviews on crystal optics readers may consult [61Ram]. To describe nonlinear optical properties related to second harmonic generation (SHG), a nonlinear susceptibility tensor is used, whose components  $d_{ijk}$  are defined by

$$P_i(2\nu) = \sum_{j,k} \varepsilon_0 d_{ijk} E_j(\nu) E_k(\nu) \quad (f)$$

in the SI (MKSA) unit system, and by

$$P_i(2\nu) = \sum_{j,k} d_{ijk} E_j(\nu) E_k(\nu) \quad (g)$$

in the cgs-esu system. Here  $P_i(2\nu)$  is a component of the second harmonic polarization of frequency  $2\nu$  generated by the electric field of light of frequency  $\nu$ ,  $E(\nu)$ , and  $\varepsilon_0$  is the dielectric permittivity of vacuum. The SHG susceptibility  $d_{i\lambda}$  is defined by  $d_{i\lambda} = d_{ijk}$  for all combinations of  $j$  and  $k$ . (For the convention on the contraction of these suffixes, see the preceding note on electromechanical and elastic properties.) Kleinman showed that the SHG susceptibility tensor may exhibit greater symmetry than the piezoelectric tensors [62Kle]. The relations deduced by him (the Kleinman conditions) are as follows:

$$d_{12} = d_{26}, \quad d_{13} = d_{35}, \quad d_{14} = d_{25} = d_{36}, \quad d_{15} = d_{31}, \quad d_{16} = d_{21}, \quad d_{23} = d_{34}, \quad d_{24} = d_{32}.$$

According to Eqs. (f) and (g),  $d_{i\lambda}$  (MKSA) has the unit of  $V^{-1} m$  and is converted to  $d_{i\lambda}$  (esu) by

$$d_{i\lambda}(\text{esu}) = \frac{3}{4\pi} \cdot 10^4 d_{i\lambda}(\text{MKSA}). \quad (h)$$

In most cases,  $d_{i\lambda}$  are given by relative values referring to  $d_{36}$  of  $\text{KH}_2\text{PO}_4$ , etc. An absolute scale recommended in [84Jer] is given below.

Material	$d_{i\lambda} [\cdot 10^{-12} V^{-1} m]$	$\lambda [\mu m]$
GaAs	$d_{14} = 134(21)$	10.6
$\text{LiIO}_3$	$d_{31} = -7.1(1.14)$	1.064
$\text{LiNbO}_3$	$d_{31} = -5.95(0.95)$	1.064
$\text{SiO}_2$	$d_{11} = 0.503(0.08)$	1.064
$\text{NH}_4\text{H}_2\text{PO}_4$	$d_{36} = 0.76(0.12)$	1.064
$\text{KH}_2\text{PO}_4$	$d_{36} = 0.63(0.1)$	1.064

For further information, readers may consult [87Eim] and [91Dmi]. It seems worthwhile giving the following comments to avoid any misconception.

- (i) The components  $P_i(2\nu)$  and  $E_j(\nu)$  stand for amplitudes of the polarization and the electric field, and not the effective values of them.
- (ii) Conversion from Eq. (f) to Eq. (g) is not made by the conventional substitution:  $\varepsilon_0 \leftrightarrow 1/4\pi$ . This is the reason why the factor  $3/(4\pi) \cdot 10^4$  appears in Eq. (h), whereas usually the conversion factor for the quantity given in  $V^{-1} m$  is  $3 \cdot 10^4$  as shown in Table IE-3.
- (iii) Although the symbol  $d_{i\lambda}$  of SHG susceptibility is the same as that of the piezoelectric strain constant, the relations between the  $d_{i\lambda}$  and the tensor component  $d_{ijk}$  are different in the two cases:  $d_{i\lambda} = d_{ijk}$  for all  $i, j, k$  in case of SHG whereas  $d_{i\lambda} = d_{ijk}$  for  $j = k$  and  $d_{i\lambda} = 2d_{ijk}$  for  $j \neq k$  in case of the piezoelectric strain constant.



### Properties studied by light scattering (10)

Scattered light gives information on elementary excitations or optical inhomogeneities in materials when they are irradiated by monochromatic light (usually laser beam). We shall use notations  $\nu_i$ ,  $\nu_s$ ,  $\mathbf{q}_i$ ,  $\mathbf{q}_s$  for  $\nu$  (frequency) and  $\mathbf{q}$  (wave number vector) of the incident and scattered lights, respectively, and  $\Delta\nu = \nu_i - \nu_s$  and  $\Delta\mathbf{q} = \mathbf{q}_i - \mathbf{q}_s$ . Naturally the unit of  $\Delta\nu$  is Hz in the SI (MKSA) unit system but in many publications the frequency shift is expressed by the wave number ( $\Delta\nu/c$ ) in vacuum in units of  $\text{cm}^{-1}$  (kayser). In this volume  $\Delta\nu$  is given in both units in most cases.

Data concerning Raman, Brillouin and Rayleigh scatterings are presented in the subsection 10 except for elastic constants which are given in the subsection 8a. In Raman scattering, the frequency shift  $\Delta\nu$  is usually caused by molecular vibrations or optical lattice vibrations. Then  $\Delta\nu$  is in general larger than  $1.5 \cdot 10^{11}$  Hz ( $5 \text{ cm}^{-1}$ ). The light scattering caused by acoustic phonons is called Brillouin scattering, for which  $\Delta\nu$  is around  $3 \cdot 10^8 \dots 1.5 \cdot 10^{11}$  Hz ( $0.01 \dots 5 \text{ cm}^{-1}$ ). There are elastic or quasielastic ( $\Delta\nu \approx 0$ ) scattering processes which are caused by inhomogeneous distribution of the refractive index in a crystal. They are called Rayleigh scattering.

The scattering geometry is expressed by a notation such as  $Z(XY)X$  for light scattering by a crystal. The notation stands for  $\mathbf{q}_i(\mathbf{e}_i, \mathbf{e}_s)\mathbf{q}_s$  where  $\mathbf{e}_i$  and  $\mathbf{e}_s$  are polarization vectors of the incident and scattered lights, respectively. Thus, the first and last letters of  $Z(XY)X$  indicate that propagation directions of the incident and scattered lights are parallel to the  $Z$  and  $X$  axes, respectively, and the two letters in parentheses indicate that polarization directions of the incident and scattered lights are parallel to the  $X$  and  $Y$  axes, respectively. Therefore,  $Z(XY)X$  corresponds to the experimental set-up illustrated in Fig. IC-1a. In case of isotropic materials (or in case the detailed specification of the scattering geometry is difficult or unnecessary), the geometry is expressed by two letters such as HV. They stand for directions of  $\mathbf{e}_i$  and  $\mathbf{e}_s$  referring to the plane determined by  $\mathbf{q}_i$  and  $\mathbf{q}_s$ . For instance, HV means that  $\mathbf{e}_i$  is horizontal (parallel) to the plane and  $\mathbf{e}_s$  is vertical (perpendicular) to the plane, as illustrated in Fig. IC-1b. Readers may consult [76Bal] or [78Hay] for details of light scattering by crystals, and [74Sco] in the relation with ferroelectrics.

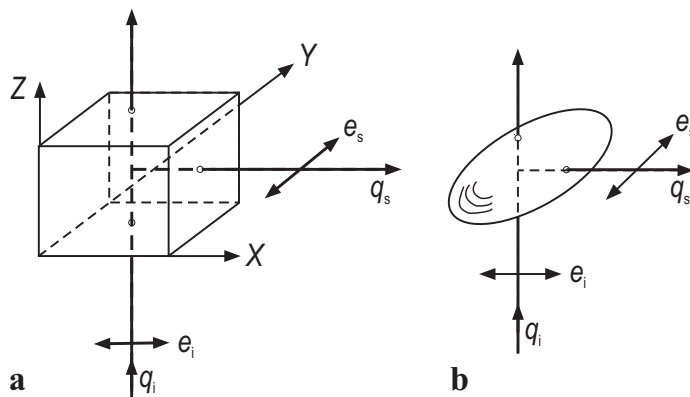


Fig. IC-1. Symbols on scattering geometries. (a)  $Z(XY)X$ . (b) HV.

Models of lattice vibrations are classified according to the irreducible representations of the 32 crystal point groups. Table IC-3 gives symbols for them together with information on their Raman and infrared activities.

When a crystal has several infrared active modes with the same symmetry, they are usually numbered by the order of increasing frequency. In this volume, the number is given as a subscript. For instance,  $E(\text{TO}_n)$  [or  $E(\text{LO}_n)$ ] is used to express the  $n^{\text{th}}$ -lowest-frequency transverse (or longitudinal) optic mode with the  $E$  symmetry.

Readers are referred to [57Kos] or [72Bra] for the mathematical theory of symmetry, and to [64Hei] for the Raman and infrared activities.

**Table IC-3. Point groups, irreducible representations, and Raman and infrared activities**

Crystal system	Point group		Irreducible representations	
	*)	**)	Raman active modes ***)	Raman inactive modes ***)
Triclinic	1	C <sub>1</sub>	A(X, Y, Z)	
	$\bar{1}$	C <sub>i</sub>	A <sub>g</sub>	A <sub>u</sub> (X, Y, Z)
Monoclinic	2	C <sub>2</sub>	A(Y), B(X, Z)	
	m	C <sub>s</sub>	A'(X, Z), A''(Y)	
	2/m	C <sub>2h</sub>	A <sub>g</sub> , B <sub>g</sub>	A <sub>u</sub> (Y), B <sub>u</sub> (X, Z)
Orthorhombic	222	D <sub>2</sub>	A, B <sub>1</sub> (Z), B <sub>2</sub> (Y), B <sub>3</sub> (X)	
	2mm	C <sub>2v</sub>	A <sub>1</sub> (Z), A <sub>2</sub> , B <sub>1</sub> (X), B <sub>2</sub> (Y)	
	mmm	D <sub>2h</sub>	A <sub>g</sub> , B <sub>1g</sub> , B <sub>2g</sub> , B <sub>3g</sub>	A <sub>u</sub> , B <sub>1u</sub> (Z), B <sub>2u</sub> (Y), B <sub>3u</sub> (X)
Tetragonal	4	C <sub>4</sub>	A(Z), B, E(X, Y)	
	$\bar{4}$	S <sub>4</sub>	A, B(Z), E(X, Y)	
	4/m	C <sub>4h</sub>	A <sub>g</sub> , B <sub>g</sub> , E <sub>g</sub>	A <sub>u</sub> (Z), B <sub>u</sub> , E <sub>u</sub> (X, Y)
	4mm	C <sub>4v</sub>	A <sub>1</sub> (Z), B <sub>1</sub> , B <sub>2</sub> , E(X, Y)	A <sub>2</sub>
	422	D <sub>4</sub>	A <sub>1</sub> , B <sub>1</sub> , B <sub>2</sub> , E(X, Y)	A <sub>2</sub> (Z)
	$\bar{4}2m$	D <sub>2d</sub>	A <sub>1</sub> , B <sub>1</sub> , B <sub>2</sub> (Z), E(X, Y)	A <sub>2</sub>
	4/mmm	D <sub>4h</sub>	A <sub>1g</sub> , B <sub>1g</sub> , B <sub>2g</sub> , E <sub>g</sub>	A <sub>2g</sub> , A <sub>1u</sub> , A <sub>2u</sub> (Z), B <sub>1u</sub> , B <sub>2u</sub> , E <sub>u</sub> (X, Y)
Trigonal	3	C <sub>3</sub>	A(Z), E(X, Y)	
	$\bar{3}$	C <sub>3i</sub>	A <sub>g</sub> , E <sub>g</sub>	A <sub>u</sub> (Z), E <sub>u</sub> (X, Y)
	32	D <sub>3</sub>	A <sub>1</sub> , E(X, Y)	A <sub>2</sub> (Z)
	3m	C <sub>3v</sub>	A <sub>1</sub> (Z), E(X, Y)	A <sub>2</sub>
	$\bar{3}m$	D <sub>3d</sub>	A <sub>1g</sub> , E <sub>g</sub>	A <sub>1u</sub> , A <sub>2u</sub> (Z), E <sub>u</sub> (X, Y)
Hexagonal	6	C <sub>6</sub>	A(Z), E <sub>1</sub> (X, Y), E <sub>2</sub>	B
	$\bar{6}$	3 <sub>2</sub> h	A', E'(X, Y), E''	A''(Z)
	6/m	C <sub>6h</sub>	A <sub>g</sub> , E <sub>1g</sub> , E <sub>2g</sub>	B <sub>g</sub> , A <sub>u</sub> (Z), E <sub>1u</sub> (X, Y), E <sub>2u</sub>
	622	D <sub>6</sub>	A <sub>1</sub> , E <sub>1</sub> (X, Y), E <sub>2</sub>	A <sub>2</sub> (Z), B <sub>1</sub> , B <sub>2</sub>
	6mm	C <sub>6v</sub>	A <sub>1</sub> (Z), E <sub>1</sub> (X, Y), E <sub>2</sub>	A <sub>2</sub> , B <sub>1</sub> , B <sub>2</sub>
	$\bar{6}m2$	D <sub>3h</sub>	A <sub>1</sub> ', E'(X, Y), E''	A <sub>2</sub> ', A <sub>1</sub> '', A <sub>2</sub> ''(Z)
	6/mmm	D <sub>6h</sub>	A <sub>1g</sub> , E <sub>1g</sub> , E <sub>2g</sub>	A <sub>2g</sub> , B <sub>1g</sub> , B <sub>2g</sub> , A <sub>1u</sub> , A <sub>2u</sub> (Z), B <sub>1u</sub> , B <sub>2u</sub> , E <sub>1u</sub> (X, Y), E <sub>2u</sub>
Cubic	23	T	A, E, F(X, Y, Z)	
	m3	T <sub>h</sub>	A <sub>g</sub> , E <sub>g</sub> , F <sub>g</sub>	A <sub>u</sub> , E <sub>u</sub> , F <sub>u</sub> (X, Y, Z)
	432	O	A <sub>1</sub> , E, F <sub>2</sub>	A <sub>2</sub> , F <sub>1</sub> (X, Y, Z)
	$\bar{4}3m$	T <sub>d</sub>	A <sub>1</sub> , E, F <sub>2</sub> (X, Y, Z)	A <sub>2</sub> , F <sub>1</sub>
	m3m	O <sub>h</sub>	A <sub>1g</sub> , E <sub>g</sub> , F <sub>2g</sub>	A <sub>2g</sub> , F <sub>1g</sub> , A <sub>1u</sub> , A <sub>2u</sub> , E <sub>u</sub> , F <sub>1u</sub> (X, Y, Z), F <sub>2u</sub>

\*) International symbol. \*\*) Schönflies symbol.

\*\*\*) Infrared active modes are indicated by adding parenthesized X, Y, Z. For instance, A(X, Y, Z) and A(Z) are infrared active whereas A<sub>g</sub> and B<sub>1g</sub> are not. The letters X, Y, Z mean that the mode is infrared active to the incident radiation polarized along the orthogonally X, Y, Z axes (cf. IC), respectively.

### Magnetic properties (12)

There are two ways to define the magnetic counterpart of the dielectric polarization  $\mathbf{P} = \mathbf{D} - \epsilon_0 \mathbf{E}$ : the magnetic polarization  $\mathbf{J} = \mathbf{B} - \mu_0 \mathbf{H}$  and the magnetization  $\mathbf{M} = \mathbf{B}/\mu_0 - \mathbf{H}$ , with  $\mathbf{J} = \mu_0 \mathbf{M}$ . In this volume magnetic properties are based upon  $\mathbf{M}$  in accordance with other Landolt-Börnstein volumes [78Nom]. Their values can be transformed into those based upon  $\mathbf{J}$  by multiplying by  $\mu_0$ .

The specific magnetization  $\sigma$  is defined by  $M/\rho$  with the unit of  $\text{Am}^2\text{kg}^{-1}$ , where  $\rho$  is the density. The molar magnetization  $\sigma_m$  is defined by  $M/(\text{mol/volume})$ .

The magnetic susceptibility  $\chi_{\text{magn}}$  is  $M/H$ . The specific susceptibility (or mass magnetic susceptibility)  $\chi_{\text{magn } \rho}$  is  $M/(H\rho)$ . The molar susceptibility  $\chi_{\text{magn } m}$  is  $M/(H(\text{mol/volume}))$ .

### Magnetic resonance and Mössbauer effect (13)

Various spin Hamiltonians used in the analysis of experimental data on ESR are listed in Table IC-4. The number assigned to each Hamiltonian in this table is used when the respective Hamiltonian is referred to in presenting data. An explanation of the spin Hamiltonian (8) is given in [64Rim]. Interpretation of other Hamiltonians can be found in [53Ble, 55Bow, 60Low, 64Hut] or [70Abr].

For general information on the Mössbauer studies, readers are referred to [63Fra] and [68Gol]. Chapters 4 and 5 of [73Bhi] are devoted to applications of Mössbauer effect to studies of lattice dynamics and ferroelectrics.

**Table IC-4. Spin Hamiltonians**

$$\mathbf{H} = \mu_B(g_x H_x S_x + g_y H_y S_y + g_z H_z S_z) \quad (1)$$

$$\mathbf{H} = g_{\perp} \mu_B(H_x S_x + H_y S_y) + g_{\parallel} \mu_B H_z S_z \quad (2)$$

$$\mathbf{H} = g_{\perp} \mu_B(H_x S_x + H_y S_y) + g_{\parallel} \mu_B H_z S_z + {}^n A_{\perp}(I_x S_x + I_y S_y) + {}^n A_{\parallel} \mathbf{I} \cdot \mathbf{S}_z \quad (3)$$

$$\mathbf{H} = g_{\perp} \mu_B(H_x S_x + H_y S_y) + g_{\parallel} \mu_B H_z S_z + D [S_z^2 - (1/3) S(S+1)] \quad (4)$$

$$\mathbf{H} = \mu_B(g_x H_x S_x + g_y H_y S_y + g_z H_z S_z) + D [S_z^2 - (1/3) S(S+1)] + E(S_x^2 - S_y^2) + {}^n \mathbf{A} \cdot \mathbf{S} \quad (5)$$

$$\mathbf{H} = \mu_B(g_x H_x S_x + g_y H_y S_y + g_z H_z S_z) + D [S_z^2 - (1/3) S(S+1)] + E(S_x^2 - S_y^2) + {}^n \mathbf{A} \cdot \mathbf{I} \quad (6)$$

$$\begin{aligned} \mathbf{H} = & g\mu_B(H_x S_x + H_y S_y + H_z S_z) + D [S_z^2 - (1/3)S(S+1)] + E(S_x^2 - S_y^2) + (F/180) [35 S^4 - 30 S(S+1) S_z^2 \\ & + 25 S_z^2 - 6S(S+1) + 3S^2(S+1)^2] + (a/6) [S_{\xi}^4 + S_{\eta}^4 + S_{\zeta}^4 - (1/5)S(S+1)(3S^2 + 3S - 1)] + {}^n \mathbf{A} \cdot \mathbf{S} \end{aligned} \quad (7)$$

$$\begin{aligned} \mathbf{H} = & g\mu_B(H_x S_x + H_y S_y + H_z S_z) + b_{20} Y_{2,0} + b_{40} [Y_{4,0} + ((70)^{1/2}/4)(Y_{4,4} + Y_{4,-4})] \\ & + b_{60} [Y_{6,0} - ((14)^{1/2}/2)(Y_{6,4} + Y_{6,-4})] + {}^n \mathbf{A} \cdot \mathbf{S} \end{aligned} \quad (8)$$

$$\mathbf{H} = g\mu_B(H_x S_x + H_y S_y + H_z S_z) + (b_{40}/60) (O_4^0 + 5 O_4^4) + (b_{60}/1260) (O_6^0 - 21 O_6^4) + {}^n \mathbf{A} \cdot \mathbf{S} \quad (9)$$

$$\mathbf{H} = \mu_B(g_x H_x S_x + g_y H_y S_y + g_z H_z S_z) + {}^n \mathbf{A} \cdot \mathbf{I} + Q_z [I_z^2 - (1/3)I(I+1)] + \sum_{\lambda} {}^n \mathbf{S} \cdot {}^n \mathbf{A}_{\lambda} \cdot \mathbf{I}_{\lambda} \quad (10)$$

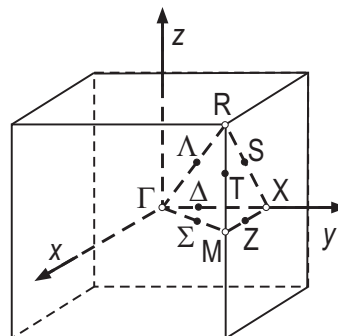
$$\mathbf{H} = \mu_B \mathbf{H} \cdot \mathbf{g} \cdot \mathbf{S} + \sum_{\lambda} {}^n \mathbf{S} \cdot {}^n \mathbf{A}_{\lambda} \cdot \mathbf{I}_{\lambda} \quad (11)$$

The summations in (10) and (11) extend over all nuclei of the ligand which are contributing to the HFS.  $Q_z$ : constants of the quadrupole interaction in the spin Hamiltonian.

### Crystal imperfections and X-ray and neutron scatterings (14)

Subsection 14 presents experimental data on temperature dependence of Bragg reflection, satellite and diffuse scatterings, and inelastic neutron scattering. They all are related with imperfections (including lattice vibrations) in the crystal. Readers may consult [62Woo], [64Gui] or [67Jam] for details of diffuse

X-ray scattering. Several conventional symbols are used to indicate special points or lines in the Brillouin zone for discussing the inelastic neutron scattering. Figure IC-2 shows them for the simple cubic lattice. Readers may consult [72Bra] or [57Kos] for other crystal lattices. Fundamentals of thermal neutron scattering are described e.g. in [65Ege], [66Bro], and [77Mar].



**Fig. IC-2.** Conventional symbols of special points in reciprocal space ( $q$ -space,  $q = 2\pi/\lambda$ ) for the simple cubic lattice.  $\Gamma$ :  $\pi/a\{0,0,0\}$ ,  $X$ :  $\pi/a\{1,0,0\}$ ,  $M$ :  $\pi/a\{1,1,0\}$ ,  $R$ :  $\pi/a\{1,1,1\}$ . The symbols  $S$ ,  $T$ ,  $Z$ ,  $\Delta$ ,  $\Lambda$ ,  $\Sigma$  represent the positions along the lines on which the filled circles sit.

#### Commensurate and incommensurate structural modulations (14)

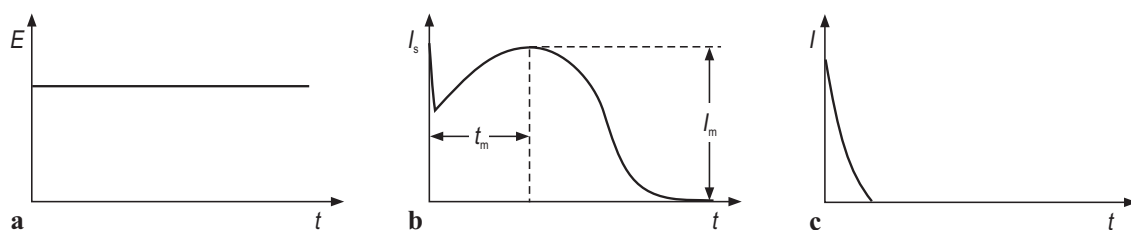
Generally molecular interaction extends over several unit cells in crystals and sometimes causes a structural modulation of long period. The modulation is called commensurate when the wave number vector  $\mathbf{k}$  ( $k = 1/\lambda$ ) of the modulation is in rational relationship with the reciprocal lattice vectors  $\mathbf{a}^*$ ,  $\mathbf{b}^*$ ,  $\mathbf{c}^*$  while the modulation is called incommensurate in irrational relationship [91Per], [92Wil]. Usually  $k$  depends upon temperature in incommensurate phases.

#### EXAFS (14)

In this volume, subsection 14 includes experimental data on EXAFS (extended X-ray absorption fine structure). Recently accurate EXAFS data are being obtained by use of the synchrotron radiation. EXAFS studies give information on local structures surrounding a specific atomic species both in crystalline and non-crystalline materials. Local structural parameters supplied by the analysis of EXAFS data are given in subsection 3b.

#### Domains (15)

Usually a ferroelectric crystal is not polarized uniformly in one direction, but is composed of many twin components which are called domains. The spontaneous polarization,  $P_s$ , is uniform within the domain. The boundary between two domains is called a wall. Some ferroelectrics (e.g. TGS) have only two possible (antiparallel) orientations of  $P_s$ , so that the domain walls separate antiparallel domains and are therefore called  $180^\circ$  walls. Other ferroelectrics (e.g.  $\text{BaTiO}_3$ ) have more than two possible orientations of  $P_s$ , and therefore a more complicated domain structure may occur. The domain wall which separates two domains having  $P_s$  at right angles to each other is called a  $90^\circ$  wall. Occasionally a crystal consists of only one domain and is called a single domain crystal. Usually, however, crystals are multi-domain crystals. A relatively strong electric field (e.g.  $100 \text{ kV m}^{-1}$ ) may change a multi-domain crystal into a single domain crystal, or may reverse the spontaneous polarization  $P_s$  of a single domain crystal. Such dynamical processes are called switching and are composed of domain wall motion and nucleation of new domains. The switching current is defined as an electric current which flows into the crystal condenser during the switching. Quantities which characterize the switching current are shown in Fig. IC-3.



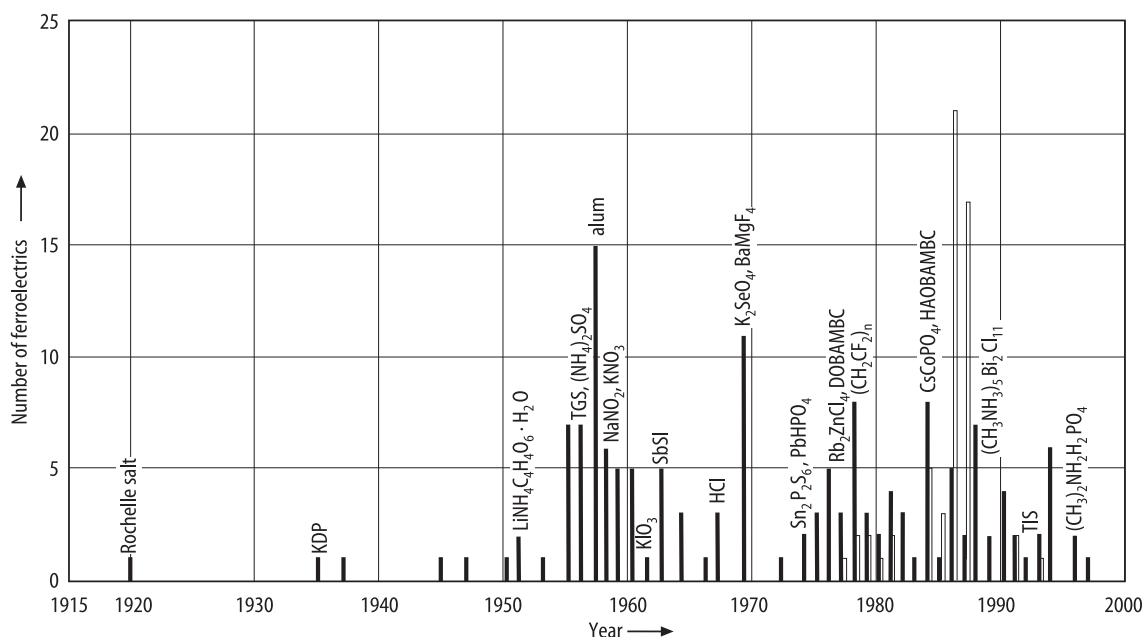
**Fig. IC-3.** Switching of ferroelectric crystal [67Fat].  $E$ : electric field strength,  $I$ : electric current,  $I_s$ : switching current,  $t$ : time. (a) constant field applied at  $t = 0$ . (b) switching current  $I_s$  obtained with an electric field antiparallel to the original  $P_s$  of the crystal.  $t_s$ : switching time,  $t_m$ : time for maximum switching current.  $I_m$ : maximum switching current. (c) Current  $I$  obtained with an electric field parallel to  $P_s$ .

### Ferroelectric thin films (16)

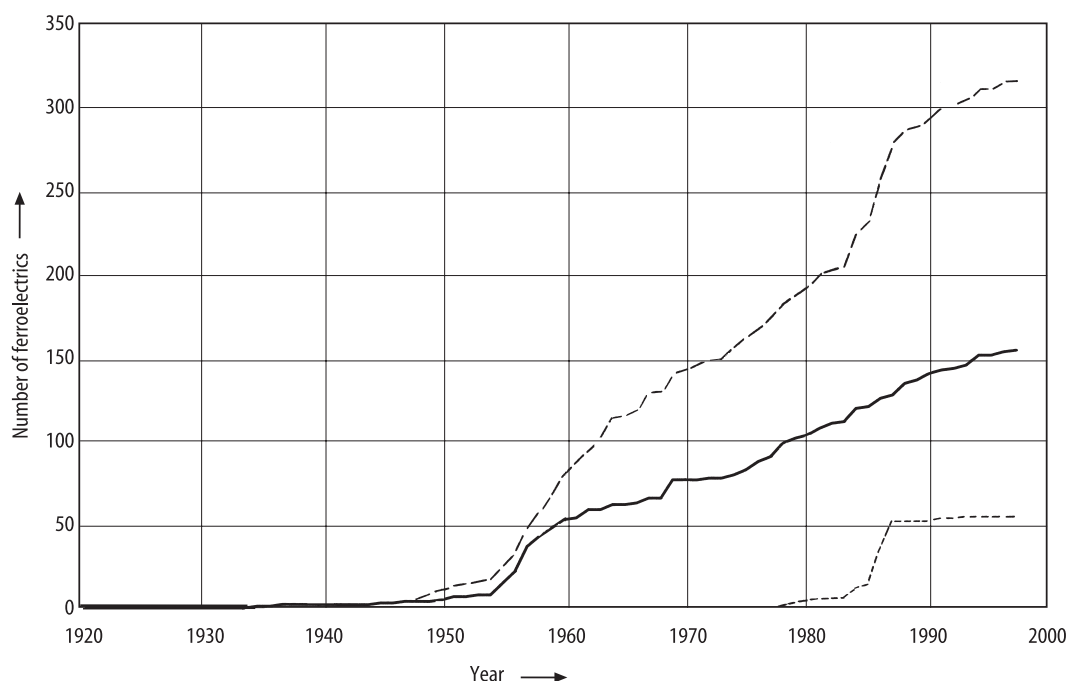
Recent advances in quantity of ferroelectric thin films have resulted in the realization of new technologies (e.g., in integrated memory devices), which were not achievable through classical bulk ceramic processing techniques. Readers may consult [96Ara], [98Sco] and the series of [95Tut] on these topics.

## ID Survey of history of ferroelectrics research

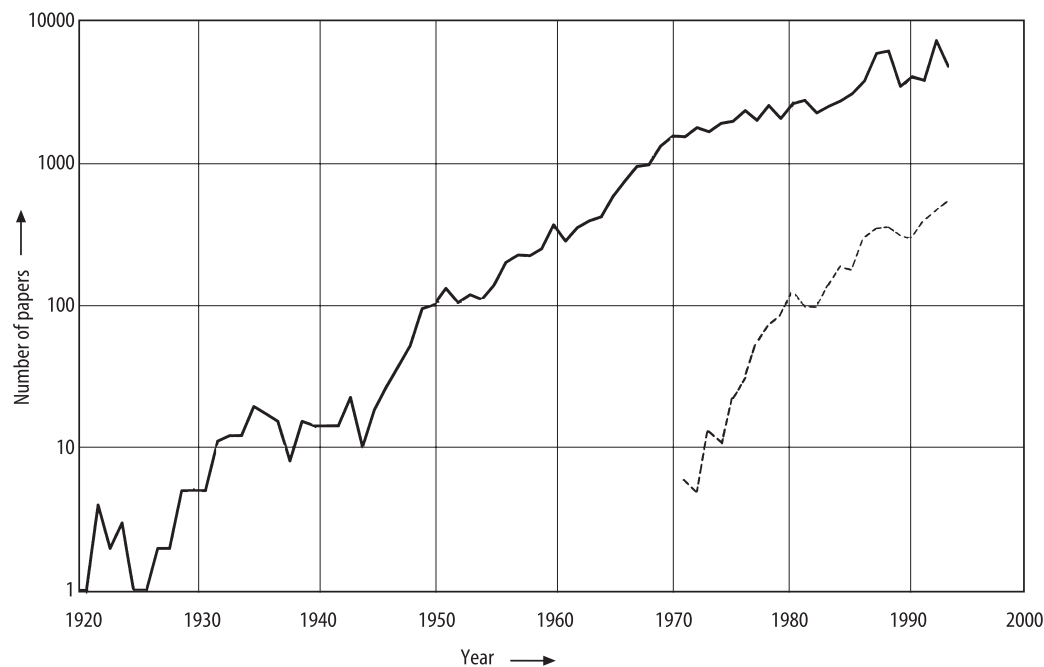
Research activities concerning ferroelectrics are increasing steadily. The situation is illustrated in Fig. ID-1, Fig. ID-2, Fig. ID-3.



**Fig. ID-1.** Number of non-oxide ferroelectrics discovered in each year. The black bar is for non-oxide crystals, counting each pure compound as one. The white bar is for liquid crystals and polymers, counting each group of homologues as one, where one group of homologues corresponds to one subsection in Chaps. 71 and 72. Representative ferroelectrics are indicated at the year of discovery. Prepared by K. Deguchi using the information given at 1a in the survey table of each section.



**Fig. ID-2.** Total numbers of non-oxide ferroelectrics and all the ferroelectrics known at the end of each year. The solid line is for non-oxide crystals, i.e., the sum of numbers indicated by black bars in Fig. ID-1. The dotted line is for liquid crystals and polymers, i.e., the sum of numbers indicated by white bars in Fig. ID-1. The dashed line is for all the ferroelectrics (oxide and non-oxide crystals + liquid crystals + polymers). Prepared by K. Deguchi on the basis of Fig. ID-1 and Fig. ID-1 in LB III/36A.



**Fig. ID-3.** Number of research papers on ferroelectrics and related substances published in each year. The solid line indicates the number for all the ferroelectrics (oxide and non-oxide crystals + liquid crystals + polymers). The dotted line indicates the number for liquid crystal and polymer ferroelectrics. Prepared by K. Deguchi on the basis of [93Toy].

## IE Symbols and units

Most symbols adopted in this volume are those which are recommended by S.U.N. Commission of IUPAP [78IUP] or used in the International Tables for X-ray Crystallography [65Lon], [83Hah], [92Wil]. The International system of units (Le Système International (SI) d'Unités) is used throughout this volume. Sometimes, however, the traditional use prefers other units for special quantities (e.g. kayser ( $\text{cm}^{-1}$ ) in optics). In such cases, the quantities are given in both SI units and traditional units in most figures and tables in this volume. An exception is Å instead of 0.1 nm. Crystallographic data are presented in Å without conversion to nm. Values of the fundamental physical constants are cited from [05Moh].

In Table IE-1, symbols used frequently in this volume are listed together with their units. In Table IE-2, symbols used as subscripts and superscripts are listed. Conversion factors from the SI (MKSA) units to the electrostatic and the electromagnetic units for important quantities are given in Table IE-3.

### Table IE-1. Symbols and units.

Symbols are arranged first in the order of the Latin alphabet and then the Greek alphabet. Such symbols as  $\Delta H$  are arranged according to the letters following  $\Delta$  (e.g.  $\Delta H$  is to be found in the place of  $H$ , not  $\Delta$ ).

#### a) Letters and signs

a, b, c, ...	Wyckoff notations for atomic positions, see [65Lon]
(hkl)	Miller indices
{hkl}	equivalent (hkl)'s in cubic or other systems
[uvw]	direction parallel to $\mathbf{r} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$ ; u, v, w: integers (referred to the $a$ , $b$ , $c$ axes of the paraelectric phase unless special remarks are made.)
<uvw>	equivalent [uvw]'s in cubic or other systems
	parallel to
⊥	perpendicular to

#### b) Abbreviations

space group international and Schoenflies symbol	LO	longitudinal optic
I, II, III, ... names of phases	LT	low temperature
A, AF antiferroelectric	mon	monoclinic
(A) possibility of being antiferroelectric	NMR	nuclear magnetic resonance
A, B, C, ... symbol for atom, various compositions	NQR	nuclear quadrupole resonance
ac alternating current	orth	orthorhombic
cub, c cubic	P	paraelectric
DTA differential thermal analysis	(P)	possibility of being paraelectric
dc direct current	pc	pseudocubic
ESR electron spin resonance	pol	polarization
EXAFS extended X-ray absorption fine structure	PTCR	positive temperature coeff. of resistance
F ferroelectric	R	Raman
(F) possibility of being ferroelectric	rh, r	rhombohedral
FS fine structure	RT	room temperature
hex, h hexagonal	SAW	surface acoustic wave
HFS hyperfine structure	SHG	second harmonic generation
HT high temperature	Sm	smectic
Im imaginary part	ss	solid solution
IR infrared	tetr	tetragonal
liq liquid	tri	trigonal
LA longitudinal acoustic	TA	transverse acoustic
	TO	transverse optic

## c) Symbols and units

Symbols	Units	Definitions
$A$	numeral	Absorption
$A$	$\text{kg kg}^{-1}$ , $\text{kg m}^{-3}$ , wt%	solubility
$A, B$	$\text{m}^{-1}$	HFS parameters
${}^n A_{ij}$	$\text{A m}^{-1}$	hyperfine splitting tensor, $n$ : nuclear mass number
${}^n A_i$	$\text{A m}^{-1}$	principal value of hyperfine splitting tensor, $n$ : nuclear mass number
${}^n A_{  }, {}^n A_{\perp}$	$\text{A m}^{-1}$	hyperfine splitting parameters in axial symmetry, $n$ : nuclear mass number
$\Delta A$	$\text{K}^{-1}$	change in slope of $1/\kappa$ vs. $T$ curve.
$a$	$\text{m}^{-1}$	FS parameter
$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\text{\AA}$	unit cell vector
$a, b, c$	$\text{\AA}$	length of unit cell edges
$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$	$\text{\AA}^{-1}$	unit cell vector in reciprocal space
$\mathbf{B}$	$\text{T} (\equiv \text{Wb m}^{-2})$ $\equiv \text{V s m}^{-2}$	magnetic induction, flux density
$B$	$\text{\AA}^2$	isotropic temperature parameter [cf. Eq. (e) in Introduction]
$B_{ij}$	numeral	anisotropic temperature parameter [cf. Eq. (a) in Introduction]
$b$	$\text{m}^{-1}$	FS parameter
$b_{ij}$	numeral	anisotropic temperature parameter [cf. Eq. (b) in Introduction]
$c$	$\text{m s}^{-1}$	light velocity in vacuum ( $c = 2.99792458 \cdot 10^8 \text{ m s}^{-1}$ )
$C$	$\text{K}$	Curie-Weiss constant with regard to $\kappa$ : $\kappa = \kappa_{\infty} + C/(T - \Theta_p)$
$C_p$	$\text{J K}^{-1} \text{ mol}^{-1}$	molar heat capacity at constant pressure
$c_p$	$\text{J K}^{-1} \text{ kg}^{-1}$	specific heat capacity at constant pressure
$c_L$	$\text{N m}^{-2}$	longitudinal elastic modulus
$c_s$	$\text{N m}^{-2}$	shear elastic modulus
$c_{\lambda\mu}$	$\text{N m}^{-2}$	elastic stiffness
$D$	$\text{m}^{-1}$	FS parameter
$D$	numeral	dissipation factor
$\mathbf{D}$	$\text{C m}^{-2}$	electric displacement
$d$	$\text{m}$	thickness of specimen
$d$	$\text{\AA}$	bond length
$d_{hkl}$	$\text{\AA}$	interplanar spacing of planes ( $hkl$ )
$d_{i\lambda}$	$\text{C N}^{-1}$	piezoelectric strain constant
$d_{i\lambda}$	$\text{m V}^{-1}$	susceptibility for second harmonic generation (see section IC)
$E$	$\text{eV}$	energy
$E$	$\text{N m}^{-2}$	Young's modulus
$E$	$\text{m}^{-1}$	FS parameter
$\mathbf{E}$	$\text{V m}^{-1}$	electric field strength
$\Delta E, \Delta E_{\text{quad}}$	$\text{m s}^{-1}$	quadrupole splitting in Mössbauer spectrum
$E_{\text{bias}}$	$\text{V m}^{-1}$	bias field
$E_c$	$\text{V m}^{-1}$	coercive field
$E_{\text{crit}}$	$\text{V m}^{-1}$	critical field
$E_G$	$\text{eV}$	energy separation, band gap
$e$	$\text{C}$	charge of electron ( $ e  = 1.602176462(63) \cdot 10^{-19} \text{ C}$ )
$\mathbf{e}$	$\text{m}^{-1}$	polarization vector of phonon
$e_{i\lambda}$	$\text{C m}^{-2}$	piezoelectric stress constant
$e^2 q Q / h$	$\text{Hz}$	nuclear quadrupole coupling constant
$e Q \phi_{ij} / h$	$\text{Hz}$	component of nuclear quadrupole coupling tensor



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Symbols	Units	Definitions
$F$	$\text{m}^{-1}$	FS parameter
$F.M._{R_I}$	$\text{C m J}^{-1}$	$F.M._{R_I} = p_i \rho^{-1} c_p^{-1}$ , figure of merit for current responsivity
$F.M._{R_V}$	$\text{C m J}^{-1}$	$F.M._{R_V} = p_i \rho^{-1} c_p^{-1} \kappa^{-1}$ , figure of merit for voltage responsivity
$F.M._N$	$\text{C m J}^{-1}$	$F.M._N = p_i \rho^{-1} c_p^{-1} \kappa^{-1/2}$ , figure of merit for material noise limited signal-to-noise ratio
$F.M._{D^*}$	$\text{Cm}^{3/2} \text{J}^{-1} \Omega^{1/2}$	$F.M._{D^*} = p_i \rho^{-1} c_p^{-1} \sigma^{-1/2}$ , figure of merit for defectivity
$f$	Hz	frequency
$f_A$	Hz	antiresonance frequency
$f_{i\lambda}$	$\text{m}^2 \text{C}^{-1}$	piezoelectric strain constant
$f_r$	Hz	dielectric relaxation frequency
$f_R$	Hz	resonance frequency
$\Delta f_R$	Hz	$f_A - f_R$
$f_R \cdot r$	Hz m	radial frequency constant
$g_i$	numeral	principal value of $g$ -tensor
$g_{ij}$	numeral	component of gyration tensor for optical activity
$g_{ij}$	numeral	component of $g$ -tensor
$g_{i\lambda}$	$\text{m}^2 \text{C}^{-1}$	piezoelectric strain constant
$H$	$\text{A m}^{-1}$	magnetic field strength
$\mathbf{H}$	$\text{J m}^{-3}$	spin Hamiltonian
$H_c$	$\text{A m}^{-1}$	coercive field strength, coercive force
$H_V$	$\text{kg m}^{-2}$	Vickers hardness number
$\Delta H$	$\text{A m}^{-1}$	magnetic resonance half width
$\Delta'H$	$\text{A m}^{-1}$	separation between maximum and minimum of the derivative of the magnetic resonance curve
$\langle \Delta H^2 \rangle$	$\text{A}^2 \text{m}^{-2}$	second moment of magnetic resonance curve
$\Delta H_{pp}$	$\text{A m}^{-1}$	line width in ESR
$\Delta H_I$	$\text{A m}^{-1}$	line shift in ESR
$\delta'H$	$\text{A m}^{-1}$	magnetic resonance line separation
$h$	J s	Planck constant ( $h = 6.6260693(11) \cdot 10^{-34} \text{ J s}$ )
$h_{i\lambda}$	$\text{N C}^{-1}$	piezoelectric stress constant
$I$	A	electric current
$I$	$\text{J s}^{-1}$	scattering intensity
$I$	numeral	nuclear spin quantum number
$I_{hkl}$	$\text{J s}^{-1}$	integrated intensity of Bragg reflection (hkl)
$I_s$	A	switching current
$J$	A	photovoltaic current
$\mathbf{J}$	$\text{V s m}^{-2}$	magnetic polarization, $\mathbf{J} = \mathbf{B} - \mu_0 \mathbf{H}$
$j$	$\text{A m}^{-2}$	electric current density
$k$	$\text{J K}^{-1}$	Boltzmann constant ( $k = 1.3806505(24) \cdot 10^{-23} \text{ J K}^{-1}$ )
$k$	$\text{m}^{-1}$	wave number vector
$k_{i\lambda}$	numeral	electromechanical coupling factor
$k_p$	numeral	planar coupling factor
$k_t$	numeral	thickness coupling factor
$L_{\lambda\mu}$	$\text{m}^2 \text{V}^{-2}$	quadratic electrooptic constant for $\mathbf{E}$
$l$	m	length
$\Delta l/l$	$\text{m m}^{-1}$	elongation per unit length
$l_{ij}$	m	coherence length
$M$	numeral	molecular weight
$\mathbf{M}$	$\text{A m}^{-1}$	magnetization, $\mathbf{M} = \mathbf{B}/\mu_0 - \mathbf{H}$

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Symbols	Units	Definitions
$M_s$	$A\ m^{-1}$	spontaneous magnetization
$M_{\lambda\mu}$	$m^4\ C^{-2}$	quadratic electrooptic constant for $\mathbf{P}$
$m_0$	kg	electron mass ( $m_0 = 9.1093826(16)\ 10^{-31}\ \text{kg}$ )
$m^*$	$m_0$	effective mass of charge carrier
$N_{\lambda\mu}$	Hz m	frequency constant
$N/N_0$	numeral	counting rate in Mössbauer spectrum
$n$	numeral	refractive index
$n_a, n_b, n_c$	numeral	refractive indices for $\mathbf{E}$ of light $\parallel a, b, c$
$n_e$	numeral	refractive index for extraordinary light
$n_o$	numeral	refractive index for ordinary light
$n_\alpha, n_\beta, n_\gamma$	numeral	principal refractive indices ( $n_\alpha < n_\beta < n_\gamma$ )
$\Delta n$	numeral	birefringence
$P$	$W\ m^{-2}$	light intensity
$P$	$C\ m^{-2}$	dielectric polarization
$P_L$	$C\ m^{-2}$	longitudinal polarization
$P_{\text{pyro}}$	$C\ m^{-2}$	pyroelectric charge
$P_r$	$C\ m^{-2}$	remanent polarization
$P_s$	$C\ m^{-2}$	spontaneous polarization
$P_w$	$C\ m^{-2}$	wing polarization
$p$	Pa	hydrostatic pressure ( $\text{Pa} = \text{N}\ m^{-2}$ )
$p$	m	helical pitch
$p_{\text{eff}}$	$\mu_B$	effective magnetic moment of atom or ion
$p_i$	$C\ K^{-1}\ m^{-2}$	pyroelectric coefficient: $p_i = \partial P_{si} / \partial T$
$p_{\lambda\mu}$	$m\ m^{-1}$	piezooptic constant for $\mathbf{S}$
$Q$	numeral	quality factor
$Q^{-1}$	numeral	internal friction
$Q_E = 1/\tan \delta$	numeral	electrical quality factor
$\Delta Q_m$	$J\ \text{mol}^{-1}$	transition heat per mole
$Q_{\lambda\mu}$	$m^4\ C^{-2}$	electrostrictive constant for $\mathbf{P}$
$q$	$m^{-1}$	wave number ( $2\pi/\lambda$ )
$\mathbf{q}$	$m^{-1}$	wave number vector
$R$	$\Omega$	resistance
$R$	numeral	reflectivity
$R$	numeral, %	discrepancy index (or reliability factor)
$R_H$	$m^3\ C^{-1}$	Hall constant
$R_M$	numeral	counting rate
$r_c$	$m\ V^{-1}$	$r_c = r_{33} - (n_o/n_e)^3 r_{13}$
$r_{\lambda i}$	$m\ V^{-1}$	electrooptic constant for $\mathbf{E}$
$S$	numeral	spin quantum number of atom or ion
$S$	$V\ K^{-1}$	Seebeck coefficient
$S$	$J\ K^{-1}\ m^{-3}$	entropy per unit volume
$S_m$	$J\ K^{-1}\ \text{mol}^{-1}$	entropy per mole
$\Delta S_m$	$J\ K^{-1}\ \text{mol}^{-1}$	transition entropy per mole
$\mathbf{S}$	$m\ m^{-1}$	strain tensor
$S_{ij}$	$m\ m^{-1}$	component of strain tensor
$S_\lambda$	$m\ m^{-1}$	component of strain tensor: $S_\lambda = S_{ij}$ for $i = j$ , $S_\lambda = 2S_{ij}$ for $i \neq j$
$s$	numeral	electron spin quantum number
$s_{\lambda\mu}$	$m^2\ N^{-1}$	elastic compliance
$T$	K, °C	temperature

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Symbols	Units	Definitions
$T$	numeral	transmission
$T_g$	K, °C	glas transition temperature
$T_{\text{melt}}$	K, °C	melting point
$T_x$	K, °C	crystallization onset temperature
$\mathbf{T}$	N m <sup>-2</sup>	stress tensor
$T_{ij}$	N m <sup>-2</sup>	component of stress tensor
$T_\lambda$	N m <sup>-2</sup>	component of stress tensor, $T_\lambda = T_{ij}$
$T_1$	sec, s	spin-lattice relaxation time
$T_{1p}$	sec, s	spin-lattice relaxation time in rotating frame
$T_2$	sec, s	spin-spin relaxation time
$\Delta T_{\text{irrev}}$	K, °C	irreversible electrocaloric temperature change
$\Delta T_{\text{rev}}$	K, °C	reversible electrocaloric temperature change
$t$	sec, s	time
$t_s$	sec, s	switching time
$t_m$	sec, s	time for maximum switching current
$\Delta U$	eV, J mol <sup>-1</sup>	activation energy
$U_{ij}$	Å <sup>2</sup>	anisotropic temperature parameter [cf. Eq. (d) in Introduction]
$V$	V	voltage
$V$	° ' ,	1/2 (optical axial angle)
$V$	Å <sup>3</sup>	volume of unit cell
$V$	° m <sup>-1</sup> T <sup>-1</sup>	Verdet constant
$V_m$	Å <sup>3</sup>	volume for formula unit
$V_\pi$	V	half-wave voltage
$V_{zz}$	V m <sup>-2</sup>	electric field gradient
$v$	m s <sup>-1</sup>	sound velocity
$v$	m s <sup>-1</sup>	velocity of absorber in Mössbauer effect
$v_0$	m s <sup>-1</sup>	effective amplitude of vibration velocity
$v_m$	m <sup>3</sup> mol <sup>-1</sup>	molar volume
$X, Y, Z$	Å, m	orthogonal coordinate system. (When $b$ is the unique axis, $Y \parallel b$ , $Z \parallel c$ and the $X$ axis forms a rectangular coordinate system together with the $Y$ and $Z$ axes.)
$x, y$	numeral	molar fraction
$x, y, z$	numeral	fractional coordinates of atoms in the unit cell
$x, y, z$	Å, m	principal axes of tensor ellipsoid
$y$	numeral	normalized yield
$Z$	numeral	number of formula units per cell
$Z_{\text{vac}}$	numeral	number of vacancies
$\alpha$	m <sup>-1</sup> , dB m <sup>-1</sup> , neper m <sup>-1</sup>	acoustic absorption coefficient
$\alpha$	dB s <sup>-1</sup>	ultrasonic attenuation
$\alpha$	m <sup>-1</sup>	optical absorption coefficient
$\alpha$	m <sup>2</sup> s <sup>-1</sup>	thermal diffusivity
$\alpha$	° ' ,	rhombohedral angle
$\alpha_{ij}$	K <sup>-1</sup>	linear thermal expansion coefficient
$\alpha_\kappa$	numeral	temperature coefficient of $\kappa$
$\alpha, \beta, \gamma$	° ' ,	interaxial angles: $b \wedge c, c \wedge a, a \wedge b$
$\alpha^*, \beta^*, \gamma^*$	° ' ,	interaxial angles: $b^* \wedge c^*, c^* \wedge a^*, a^* \wedge b^*$
$\beta_{ij}$	Å <sup>2</sup>	anisotropic temperature parameter [cf. Eq. (c) in Introduction]

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Symbols	Units	Definitions
$\Gamma$	Hz	full width at half maximum of spectral line
$\Gamma$	Hz	damping parameter
$\Gamma$	$\text{m s}^{-1}$	line width of Mössbauer absorption line (half width at half maximum)
$\gamma$	$\text{m A}^{-1} \text{ s}^{-1}$	gyromagnetic ratio
$\gamma$	$\text{K}^{-1}$	cubic thermal expansion coefficient
$\delta$	$\text{m s}^{-1}$	isomer shift
$\delta$	rad	dielectric loss angle
$\tan \delta$	numeral	dielectric loss tangent: $\tan \delta = \kappa''/\kappa'$
$\varepsilon$	$\text{F m}^{-1}$	permittivity, $D = \varepsilon E$
$\varepsilon_{ij}$	$\text{F m}^{-1}$	components of dielectric permittivity tensor
$\varepsilon_0$	$\text{F m}^{-1}$	permittivity of vacuum ( $\varepsilon_0 = 8.854187817 \cdot 10^{-12} \text{ F m}^{-1}$ )
$\zeta$	$\text{V m}^9 \text{ C}^{-5}$	coefficient of power series expansion of electric field strength: $E = (1/\chi_p)P + \xi P^3 + \zeta P^5$
$\zeta$	numeral	reduced wave vector coordinate
$\eta$	numeral	asymmetry parameter
$\theta$	K, °C	transition temperature
$\theta_{\text{II-I}}$	K, °C	transition temperature between the phases II and I
$\theta_c$	K, °C	superconducting transition temperature
$\theta_f$	K, °C	ferroelectric transition temperature
$\theta_a$	K, °C	antiferroelectric transition temperature
$\theta_p$	K, °C	paraelectric Curie temperature in the Curie-Weiss law
$\theta_{\text{f magn}}$	K, °C	ferromagnetic transition temperature
$\theta_N$	K, °C	antiferromagnetic Néel temperature
$\theta_{\text{p magn}}$	K, °C	paramagnetic Curie temperature in the Curie-Weiss law
$\theta_\phi$	K, °C	phase match temperature
$\Delta\theta$	K, °C	shift of phase transition temperature
$\theta$	°	tilt angle
$\theta_B$	rad, °	Bragg angle (scattering angle = $2\theta_B$ )
$\kappa$	numeral	dielectric constant: $\kappa = \varepsilon/\varepsilon_0$
$\kappa_0$	numeral	static dielectric constant
$\kappa_\infty$	numeral	temperature-independent term in Curie-Weiss law: $\kappa = \kappa_\infty + C/(T - \theta_p)$
$\kappa', \kappa''$	numeral	real and imaginary parts of complex dielectric constant: $\kappa = \kappa' + i\kappa''$
$\kappa_{ij}$	numeral	component of dielectric constant tensor
$\kappa_{[\text{uvw}]}$	numeral	dielectric constant for $\mathbf{E} \parallel [\text{uvw}]$
$\kappa_{(\text{hkl})}$	numeral	dielectric constant of crystal cut parallel to (hkl)
$\kappa_a, \kappa_b, \kappa_c$	numeral	dielectric constant along the $a, b, c$ axes
$\lambda$	m	wave length
$\lambda$	$\text{J s}^{-1} \text{ m}^{-1} \text{ K}^{-1}$	thermal conductivity
$1/\lambda$	$\text{m}^{-1}$	wave number per unit length
$\lambda, \mu, \nu$	numeral	direction cosines
$\mu_0$	$\text{H m}^{-1}$	permeability of vacuum ( $\mu_0 = 4\pi \cdot 10^{-7} \text{ H m}^{-1}$ )
$\mu_B$	$\text{J T}^{-1}$	Bohr magneton ( $\mu_B = 9.27400949(80) \cdot 10^{-24} \text{ J T}^{-1}$ )
$\mu_n$	$\text{J T}^{-1}$	nuclear magneton ( $\mu_n = 5.05078343(43) \cdot 10^{-27} \text{ J T}^{-1}$ )
$\mu_H$	$\text{m}^2 \text{ V}^{-1} \text{ s}^{-1}$	Hall mobility
$\nu$	Hz	frequency (mainly used in optical properties)
$\Delta\nu$	Hz	splitting of the resonance frequencies
$\Delta\nu$	Hz	frequency shift

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Symbols	Units	Definitions
$\nu_{\text{H}}$	Hz	frequency of resonance field
$\nu_{\text{L}}$	Hz	Larmor frequency
$\nu_{\text{c}}$	Hz	correlation frequency
$\delta\nu$	Hz	half width at half maximum
$\delta\nu$	Hz	doublet separation of NQR spectrum
$\xi$	$\text{V m}^5 \text{C}^{-3}$	coefficient of power series expansion of electric field strength: $E = (1/\chi_{\text{p}})P + \xi P^3 + \zeta P^5$
$\xi, \eta, \zeta$	numeral	fractional coordinates in the reciprocal unit cell
$I_{\lambda\mu}$	$\text{m}^2 \text{N}^{-1}$	piezooptic constant for <b>T</b>
$\pi_{i\lambda}$	$\text{m}^2 \text{N}^{-1}$	piezoresistive constant
$\rho$	$\Omega \text{m}$	resistivity
$\rho$	$^\circ \text{m}^{-1}$	specific rotatory power
$\rho$	$\text{kg m}^{-3}$	density
$\rho_{\text{a}}$	$\text{kg m}^{-3}$	apparent density
$\rho_{\text{e}}$	$\text{\AA}^{-3}$	electron density (number of electrons per $\text{\AA}^3$ )
$\rho_{\text{r}}$	$\text{kg m}^{-3}$	relative density
$\rho_{\text{X}}$	$\text{kg m}^{-3}$	X-ray density
$\rho_{\lambda i}$	$\text{m}^2 \text{C}^{-1}$	electrooptic constant for <b>P</b>
$\sigma$	$\Omega^{-1} \text{m}^{-1}$	conductivity
$\sigma$	$\Omega^{-1}$	surface conductivity
$\sigma$	$\text{C m}^{-1}$	charge density
$\sigma$	numeral	standard deviation in fractional coordinates of atomic position
$\sigma$	$\text{\AA}^2$	standard deviation in temperature parameter
$\sigma$	$\text{A m}^2 \text{kg}^{-1}$	magnetic moment per unit mass, specific magnetization
$\sigma_{\text{m}}$	$\text{A m}^2 \text{mol}^{-1}$	magnetic moment per mole
$\sigma_{\text{ph}}$	$\Omega^{-1} \text{m}^{-1}$	photoconductivity
$\tau$	sec, s	dielectric relaxation time
$\tau_{\text{c}}$	sec, s	correlation time
$\phi$	$^\circ, '$	rotation angle
$\phi_{\text{o}}$	$^\circ, '$	rotation angle of optical indicatrix
$\phi_{ij}$	$\text{V m}^{-2}$	components of the electric field gradient tensor
$\chi$	$\text{F m}^{-1}$	electric susceptibility
$\chi_{\text{p}}$	$\text{F m}^{-1}$	paraelectric susceptibility
$\chi_{\text{magn m}}$	$\text{m}^3 \text{mol}^{-1}$	molar magnetic susceptibility
$\chi_{\text{magn } \rho}$	$\text{m}^3 \text{kg}^{-1}$	mass magnetic susceptibility, specific susceptibility
$\chi_{\text{me}}$	$\text{s m}^{-1}$	magnetoelectric susceptibility

**Table IE-2. Subscripts and superscripts arranged alphabetically**

Superior	Definitions	Superior	Definitions
0	at 0 K	<i>S</i>	at entropy <i>S</i> (adiabatic)
numeral (left)	mass number	<b>S</b>	at strain <b>S</b>
<b>D</b>	at electric displacement <b>D</b>	<i>T</i>	at temperature <i>T</i>
<b>E</b>	at field strength <b>E</b>	<b>T</b>	at stress <b>T</b>
<b>P</b>	at polarization <b>P</b>		

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Inferior	Definitions	Inferior	Definitions
a	antiferroelectric	crit	critical
<i>a, b, c</i>	parallel to the <i>a, b, c</i> axes	cub, c	cubic
A, B, a, b, c, ...	sublattice A, B, a, b, c, ...	det	determined
d	diffuse	dia	diamagnetic
e	extraordinary light	eff	effective
f	ferroelectric	exp	experimental
g	per gram (only for magnetic quantities)	ext	external
HT	high temperature	fmagn	ferromagnetic
i, j, k	numerals (1...3)	hex, h	hexagonal
$\lambda, \mu, \nu$	numerals (1...6)	int	internal
LT	low temperature	loc	local
m	per mole; per molecule; maximum (in a few cases)	magn	magnetic
n	nuclear, per nucleus	max	maximum
n	normalized	me	magnetoelectric
o	ordinary light	mech	mechanical
p	paraelectric	melt	melting
<i>p</i>	at pressure <i>p</i>	min	minimum
R	resonance	mon	monoclinic
r	remanent	obs	observed
s	spontaneous; switching	orth	orthorhombic
<i>v</i>	at volume <i>v</i>	pmagn	paramagnetic
[uvw]	parallel to the [uvw] direction	prk	perovskite
(hkl)	perpendicular to the (hkl) plane	ps	pseudo
	parallel	pyro	pyroelectric
⊥	perpendicular	quad	quadrupole
amagn	antiferromagnetic	res	resonance
anis	anisotropic	rh, r	rhombohedral
brk	breakdown	sol	solid
calc	calculated	tetr	tetragonal
		th	theoretical
		thr	threshold

**Table IE-3. Conversion factors from the SI system to the cgs-esu and the cgs-emu systems**

(Replace the value of column 3 by the value of column 4 or column 5). Arrangement is made according to the order of the properties of Table IE-1.

Quantities	Symbols	SI	cgs-esu (non-rationalized)	cgs-emu
Length	<i>l</i>	m	10 <sup>2</sup> cm	10 <sup>2</sup> cm
Mass	<i>m</i>	kg	10 <sup>3</sup> g	10 <sup>3</sup> g
Time	<i>t</i>	s	1 s	1 s
Density	$\rho$	kg m <sup>-3</sup>	10 <sup>-3</sup> g cm <sup>-3</sup>	10 <sup>-3</sup> g cm <sup>-3</sup>
Electric field strength	<i>E</i>	V m <sup>-1</sup>	10 <sup>-4</sup> / 3 esu	10 <sup>6</sup> emu
Electric displacement	<b><i>D</i></b>	C m <sup>-2</sup>	12 $\pi$ ·10 <sup>5</sup> esu	4 $\pi$ ·10 <sup>-5</sup> emu
Dielectric polarization	<b><i>P</i></b>	C m <sup>-2</sup>	3·10 <sup>5</sup> esu	10 <sup>-5</sup> emu
Dielectric constant	$\kappa$	dimensionless	1 (dimensionless)	1 (dimensionless)
Piezooptic constant	<i>p</i> <sub><math>\lambda\mu</math></sub>	dimensionless	1 (dimensionless)	1 (dimensionless)

(continued)

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Table IE-3 (continued)

Quantities	Symbols SI	cgs-esu (non-rationalized)	cgs-emu
Electric susceptibility	$\chi$ F m <sup>-1</sup>	9·10 <sup>9</sup> (dimensionless)	10 <sup>-11</sup> emu
Pyroelectric coefficient	$p_i$ C m <sup>-2</sup> K <sup>-1</sup>	3·10 <sup>5</sup> esu K <sup>-1</sup>	10 <sup>-5</sup> emu K <sup>-1</sup>
Electric current density	$j$ A m <sup>-2</sup>	3·10 <sup>5</sup> esu	10 <sup>-5</sup> emu
Resistivity	$\rho$ $\Omega$ m	10 <sup>-9</sup> / 9 esu	10 <sup>11</sup> emu
Conductivity	$\sigma$ $\Omega^{-1}$ m <sup>-1</sup>	9·10 <sup>9</sup> esu	10 <sup>-11</sup> emu
Molar heat capacity at constant pressure	$C_p$ J K <sup>-1</sup> mol <sup>-1</sup>	10 <sup>7</sup> erg K <sup>-1</sup> mol <sup>-1</sup>	10 <sup>7</sup> erg K <sup>-1</sup> mol <sup>-1</sup>
Transition heat per mole	$\Delta Q_m$ J mol <sup>-1</sup>	10 <sup>7</sup> erg mol <sup>-1</sup>	10 <sup>7</sup> erg mol <sup>-1</sup>
Transition entropy per mole	$\Delta S_m$ J K <sup>-1</sup> mol <sup>-1</sup>	10 <sup>7</sup> erg K <sup>-1</sup> mol <sup>-1</sup>	10 <sup>7</sup> erg K <sup>-1</sup> mol <sup>-1</sup>
Thermal conductivity	$\lambda$ J m <sup>-1</sup> s <sup>-1</sup> K <sup>-1</sup>	10 <sup>5</sup> erg cm <sup>-1</sup> s <sup>-1</sup> K <sup>-1</sup>	10 <sup>5</sup> erg cm <sup>-1</sup> s <sup>-1</sup> K <sup>-1</sup>
Stress tensor	$\mathbf{T}$ N m <sup>-2</sup>	10 dyn cm <sup>-2</sup>	10 dyn cm <sup>-2</sup>
Hydrostatic pressure	$p$ Pa (= N m <sup>-2</sup> )	10 dyn cm <sup>-2</sup>	10 dyn cm <sup>-2</sup>
Strain tensor	$\mathbf{S}$ m m <sup>-1</sup>	1 cm cm <sup>-1</sup>	1 cm cm <sup>-1</sup>
Elastic stiffness	$c_{\lambda\mu}$ N m <sup>-2</sup>	10 dyn cm <sup>-2</sup>	10 dyn cm <sup>-2</sup>
Elastic compliance	$s_{\lambda\mu}$ m <sup>2</sup> N <sup>-1</sup>	10 <sup>-1</sup> cm <sup>2</sup> dyn <sup>-1</sup>	10 <sup>-1</sup> cm <sup>2</sup> dyn <sup>-1</sup>
Piezoelectric strain constant	$d_{i\lambda}$ C N <sup>-1</sup>	3·10 <sup>4</sup> esu	10 <sup>-6</sup> emu
Piezoelectric stress constant	$e_{i\lambda}$ C m <sup>-2</sup>	3·10 <sup>5</sup> esu	10 <sup>-5</sup> emu
Piezoelectric strain constant	$g_{i\lambda}$ m <sup>2</sup> C <sup>-1</sup>	10 <sup>-5</sup> / 3 esu	10 <sup>5</sup> emu
Piezoelectric stress constant	$h_{i\lambda}$ N C <sup>-1</sup>	10 <sup>-4</sup> / 3 esu	10 <sup>6</sup> emu
Electrostrictive constant (for $\mathbf{P}$ )	$Q_{\lambda\mu}$ m <sup>4</sup> C <sup>-2</sup>	10 <sup>-10</sup> / 9 esu	10 <sup>10</sup> emu
Electrooptic constant (for $\mathbf{P}$ )	$\rho_{i\lambda}$ m <sup>2</sup> C <sup>-1</sup>	10 <sup>-5</sup> / 3 esu	10 <sup>5</sup> emu
Electrooptic constant (for $\mathbf{E}$ )	$r_{i\lambda}$ m V <sup>-1</sup>	3·10 <sup>4</sup> esu	10 <sup>-6</sup> emu
Piezooptic constant (for $\mathbf{T}$ )	$I\Gamma_{\lambda\mu}$ m <sup>2</sup> N <sup>-1</sup>	10 <sup>-1</sup> cm <sup>2</sup> dyn <sup>-1</sup>	10 <sup>-1</sup> cm <sup>2</sup> dyn <sup>-1</sup>
Quadratic electrooptic constant (for $\mathbf{E}$ )	$L_{\lambda\mu}$ m <sup>2</sup> V <sup>-2</sup>	9·10 <sup>8</sup> esu	10 <sup>-12</sup> emu
Quadratic electrooptic constant (for $\mathbf{P}$ )	$M_{\lambda\mu}$ m <sup>4</sup> C <sup>-2</sup>	10 <sup>-10</sup> / 9 esu	10 <sup>10</sup> emu
Hall constant	$R_H$ m <sup>3</sup> C <sup>-1</sup>	10 <sup>-3</sup> / 3 esu	10 <sup>7</sup> emu
Magnetic induction (flux density)	$\mathbf{B}$ T ( $\equiv$ Wb m <sup>-2</sup> $\equiv$ V s m <sup>-2</sup> )	10 <sup>-6</sup> / 3 esu	10 <sup>4</sup> G
Magnetic field	$\mathbf{H}$ A m <sup>-1</sup>	12 $\pi$ ·10 <sup>7</sup> esu	4 $\pi$ ·10 <sup>-3</sup> Oe
Magnetic polarization ( $\mathbf{B} = \mu_0 \mathbf{H} + \mathbf{J}$ )	$\mathbf{J}$ T ( $\equiv$ Wb m <sup>-2</sup> $\equiv$ V s m <sup>-2</sup> )	10 <sup>-6</sup> / (12 $\pi$ ) esu	10 <sup>4</sup> / (4 $\pi$ ) G
Magnetization ( $\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M})$ )	$\mathbf{M}$ A m <sup>-1</sup>	3·10 <sup>7</sup> esu	10 <sup>-3</sup> G
Magnetic moment per unit mass, specific magnetization	$\sigma$ A m <sup>2</sup> kg <sup>-1</sup>	3·10 <sup>10</sup> esu cm <sup>3</sup> g <sup>-1</sup>	1 emu g <sup>-1</sup>
Magnetic moment per mole	$\sigma_m$ A m <sup>2</sup> mol <sup>-1</sup>	3·10 <sup>13</sup> esu cm <sup>3</sup> mol <sup>-1</sup>	10 <sup>3</sup> emu mol <sup>-1</sup>
Mass magnetic susceptibility, specific susceptibility	$\chi_{\text{magn } \rho}$ m <sup>3</sup> kg <sup>-1</sup>	10 <sup>3</sup> / (4 $\pi$ ) esu cm <sup>3</sup> g <sup>-1</sup>	10 <sup>3</sup> / (4 $\pi$ ) emu g <sup>-1</sup>
Molar magnetic susceptibility	$\chi_{\text{magn } m}$ m <sup>3</sup> mol <sup>-1</sup>	10 <sup>6</sup> / (4 $\pi$ ) esu cm <sup>3</sup> mol <sup>-1</sup>	10 <sup>6</sup> / (4 $\pi$ ) emu mol <sup>-1</sup>
Magnetic susceptibility	$\chi_{\text{magn}}$ dimensionless	1 / (4 $\pi$ ) dimensionless	1 / (4 $\pi$ ) dimensionless
Magnetic resonance half width	$\Delta H$ A m <sup>-1</sup>	12 $\pi$ ·10 <sup>7</sup> esu	4 $\pi$ ·10 <sup>-3</sup> Oe
Second moment of magnetic resonance curve	$\langle \Delta H^2 \rangle$ A <sup>2</sup> m <sup>-2</sup>	144 $\pi^2$ ·10 <sup>14</sup> esu	16 $\pi^2$ ·10 <sup>-6</sup> Oe
Gyromagnetic ratio	$\gamma$ m A <sup>-1</sup> s <sup>-1</sup>	10 <sup>-7</sup> / (12 $\pi$ ) esu	10 <sup>3</sup> / (4 $\pi$ ) Oe <sup>-1</sup> s <sup>-1</sup>
Isomer shift	$\delta$ m s <sup>-1</sup>	10 <sup>2</sup> cm s <sup>-1</sup>	10 <sup>2</sup> cm s <sup>-1</sup>
Magnetoelectric susceptibility	$\chi_{\text{me}}$ s m <sup>-1</sup>	10 <sup>-2</sup> / (4 $\pi$ ) s cm <sup>-1</sup>	10 <sup>-2</sup> / (4 $\pi$ ) s cm <sup>-1</sup>

## IF Survey of contained data

Each chapter of this volume corresponds to one family consisting of similar substances. This Sub-volume B contains 30 families of inorganic substances other than oxides and thus 30 chapters, as listed in Table IG-1. Each section in a chapter is devoted to describing properties of one substance (pure compound or solid solution). Table IF-1 shows how the data are presented in each section: A section is divided into 16 subsections and each subsection gives the data on special properties (e.g., dielectric properties). The information given in each section is surveyed by a table at the beginning of the section according to the order of subsections 1...16 of Table IF-1.

A detailed two-dimensional survey of contained data is made in Table IF-2 which gives all the substances appearing in the subvolumes B along the ordinate and properties along the abscissa.

**Table IF-1. Arrangement of data for each substance**

Subsection	Information
1	History and fundamental quantities.
a	History (discoverer, year of discovery).
b	Fundamental quantities (phases, state (F, A, P), crystal system, space group of each phase, transition temperatures, direction of spontaneous polarization, melting point, density, transparency and color, cleavage plane, deliquescence and efflorescence, phase diagram for solid solution).
2	Material preparation and crystal growth.
a	Method, solubility in fluxes or solvents.
b	Crystal forms, <i>a</i> , <i>b</i> , <i>c</i> axes, <i>X</i> , <i>Y</i> , <i>Z</i> axes.
3	Crystal structure.
a	Unit cell parameters.
b	Crystal structure ( <i>Z</i> , table of positional and temperature parameters, interatomic distances and bond angles, figure of crystal structures, structural change associated with phase transitions).
4	Lattice distortions (thermal expansion, lattice deformation associated with spontaneous polarization).
5	Dielectric properties.
a	Dielectric constants ( $\kappa$ vs. <i>T</i> , Curie-Weiss law constants, $\kappa$ vs. <i>p</i> , $\kappa$ vs. two- or one-dimensional pressure, $\kappa$ vs. frequency, phase diagram in regard to <i>p</i> and $E_{\text{bias}}$ ).
b	Nonlinear dielectric properties (effect of $E_{\text{bias}}$ on $\kappa$ ; values of $\xi$ and $\zeta$ ).
c	Spontaneous polarization and coercive field (or critical field for antiferroelectrics).
d	Pyroelectric and electrocaloric effect.
6	Thermal properties.
a	Heat capacity, transition heat, transition entropy.
b	Thermal conductivity.
7	Electromechanical properties.
a	Piezoelectricity.
b	Electrostriction.
c	Nonlinear electromechanical properties.

(continued)



## I Introduction

Table IF-1 (continued)

Subsection	Information
8	Elastic properties.
a	Elastic compliances and stiffnesses (including data on acoustic surface wave).
b	Nonlinear elastic properties.
9	Optical properties.
a	Refractive indices, birefringence, reflection, absorption (infrared region, visible region, ultraviolet region).
b	Electrooptic effect.
c	Piezoelectric effect (photoelastic effect).
d	Optical activity (rotatory power), Faraday effect.
e	Nonlinear optical properties.
10	Properties studied by light scattering.
a	Raman scattering.
b	Brillouin scattering and Rayleigh scattering. (Elastic constants are given in 8a.)
11	Electrical conduction (conductivity, breakdown strength, thermoelectric effect, photoconductivity and photoemission, superconductivity, band structure).
12	Magnetic properties (magnetic susceptibility, spontaneous magnetization, magnetic structure, magnetoelectric effect).
13	Properties studied by magnetic resonance and Mössbauer effect.
a	NMR.
b	ESR and ENDOR.
c	Mössbauer effect.
14	Diffraction phenomena related with secondary structures and local structures.
a	Bragg reflections due to structural modulations.
b	Diffuse or inelastic scattering.
c	EXAFS.
15	Domains.
a	Domain structure.
b	Effects of electric field and mechanical stress.
16	Miscellanea (thin layer, surface layer, radiation damage, plasticity, dislocation, etchant, point defects, twin structure, stripe pattern, paraelectric resonance).

**Table IF-2. Two-dimensional survey of contained data**

This table indicates the pages where the required data for special properties and individual substances can be found. All the substances appearing in the subvolumes III/36B are given along the ordinate and properties along the abscissa. More detailed information on the properties can be found in Table IF-1. Abbreviations in this table: [F]: ferroelectric. [(F)]: possibility of ferroelectricity. [A]: antiferroelectric. [(A)]: possibility of antiferroelectricity.

Subvolume III/36B1		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellanea
No.	Substance																	
20 SbSI family																		
20A Pure compounds																		
1	BiSCl	20A-01	•	•	•							•	•	•				
2	BiSeCl	20A-02	•		•								•					
3	SbSBr [F]	20A-03	•	•	•		•	•			•	•	•	•	•	•		
4	BiSBr [F]	20A-04	•	•	•		•					•	•					
5	SbSeBr	20A-05	•	•	•								•					
6	BiSeBr	20A-06	•	•	•								•	•				
7	SbSI [F]	20A-07	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
8	BiSI [F]	20A-08	•	•	•		•	•			•		•	•	•			
9	SbSeI	20A-09	•	•	•		•	•		•	•		•	•	•			
10	BiSeI	20A-10	•	•	•						•		•	•				
11	SbTeI	20A-11	•	•	•						•		•		•			
20B Solid solutions																		
1	SbSBr–SbSI	20B-01	•	•	•		•					•						
2	SbSI–SbOI	20B-02	•	•														
3	SbSI–AsSI	20B-03	•	•			•				•	•						
4	SbSI–BiSI	20B-04	•	•			•					•						
5	SbSI–SbSeI	20B-05	•		•	•	•				•		•					
21 TlS																		
21A Pure compound																		
1	TlS [F]	21A-01	•	•	•		•	•					•					
22 TlInS <sub>2</sub> family																		
22A Pure compounds																		
1	TlGaS <sub>2</sub>	22A-01	•	•	•	•	•	•			•	•	•					
2	TlInS <sub>2</sub> [F]	22A-02	•	•	•	•	•			•	•	•	•			•		
3	TlGaSe <sub>2</sub> [F]	22A-03	•	•	•		•	•			•	•	•					

Subvolume III/36B1		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellanea
No.	Substance																	
4	TlInSe <sub>2</sub>	22A-04	•		•							•						
5	TlSbSe <sub>2</sub>	22A-05					•											
<b>22B Solid solutions</b>																		
1	TlInS <sub>2</sub> –TlFeSe <sub>2</sub>	22B-01					•											
2	TlInS <sub>2</sub> –TlInSe <sub>2</sub>	22B-02					•				•		•					
3	TlGaSe <sub>2</sub> –TlFeSe <sub>2</sub>	22B-03					•											
4	TlGaS <sub>2</sub> –AgGaS <sub>2</sub>	22B-04				•												
5	TlInS <sub>2</sub> –CuInS <sub>2</sub>	22B-05				•												
<b>23 Ag<sub>3</sub>AsS<sub>3</sub> family</b>																		
<b>23A Pure compounds</b>																		
1	Ag <sub>3</sub> AsS <sub>3</sub> [F]	23A-01	•	•	•	•	•	•		•	•	•	•		•	•	•	•
2	Ag <sub>3</sub> SbS <sub>3</sub>	23A-02	•	•	•		•		•	•	•	•	•		•			
<b>23B Solid solution</b>																		
1	Ag <sub>3</sub> AsS <sub>3</sub> –Ag <sub>3</sub> SbS <sub>3</sub>	23B-01									•							
<b>24 Sn<sub>2</sub>P<sub>2</sub>S<sub>6</sub> family</b>																		
<b>24A Pure compounds</b>																		
1	Sn <sub>2</sub> P <sub>2</sub> S <sub>6</sub> [F]	24A-01	•	•	•	•	•	•	•	•	•	•	•			•	•	•
2	Sn <sub>2</sub> P <sub>2</sub> Se <sub>6</sub> [(F)]	24A-02	•	•	•	•	•	•		•	•	•			•	•		
<b>24B Solid solutions</b>																		
1	Sn <sub>2</sub> P <sub>2</sub> S <sub>6</sub> –Pb <sub>2</sub> P <sub>2</sub> S <sub>6</sub>	24B-01	•		•		•					•			•			
2	Sn <sub>2</sub> P <sub>2</sub> Se <sub>6</sub> –Pb <sub>2</sub> P <sub>2</sub> Se <sub>6</sub>	24B-02	•		•		•				•							
3	Sn <sub>2</sub> P <sub>2</sub> S <sub>6</sub> –Sn <sub>2</sub> P <sub>2</sub> Se <sub>6</sub>	24B-03	•		•		•	•								•		
<b>25 KNiCl<sub>3</sub> family</b>																		
<b>25A Pure compounds</b>																		
1	KNiCl <sub>3</sub> [F]	25A-01	•	•	•		•								•	•		

Subvolume III/36B1		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellanea
No.	Substance																	
2	RbFeBr <sub>3</sub> [F]	25A-02	•	•	•		•											
3	RbMnBr <sub>3</sub> [F]	25A-03	•	•	•		•				•							
<b>26 BaMnF<sub>4</sub> family</b>																		
<b>26A Pure compounds</b>																		
1	BaMgF <sub>4</sub> [F]	26A-01	•	•	•	•	•		•	•	•				•			
2	BaMnF <sub>4</sub> [(F)]	26A-02	•	•	•	•	•	•	•	•	•	•	•	•	•	•		
3	BaFeF <sub>4</sub> [(F)]	26A-03	•	•	•		•						•	•				
4	BaCoF <sub>4</sub> [F]	26A-04	•	•	•		•							•				
5	BaNiF <sub>4</sub> [F]	26A-05	•	•	•		•							•	•			
6	BaZnF <sub>4</sub> [F]	26A-06	•	•	•		•				•	•		•				
<b>27 HCl family</b>																		
<b>27A Pure compounds</b>																		
1	HCl [F]	27A-01	•	•	•	•	•	•		•	•	•			•	•		
2	HBr [F]	27A-02	•	•	•	•	•	•		•	•	•			•	•		
<b>28 NaNO<sub>2</sub> family</b>																		
<b>28A Pure compounds</b>																		
1	NaNO <sub>2</sub> [F]	28A-01	•	•	•	•	•	•	•	•	•	•	•		•	•	•	•
2	AgNa(NO <sub>2</sub> ) <sub>2</sub> [F]	28A-02	•	•	•	•	•	•	•	•	•	•	•		•		•	
<b>28B Solid solutions</b>																		
1	NaNO <sub>2</sub> –AgNO <sub>2</sub>	28B-01	•															
2	NaNO <sub>2</sub> –NaNO <sub>3</sub>	28B-02	•				•											
<b>29 CsCd(NO<sub>2</sub>)<sub>3</sub> family</b>																		
<b>29A Pure compounds</b>																		
1	RbCd(NO <sub>2</sub> ) <sub>3</sub> [(F)]	29A-01	•	•	•		•										•	
2	CsCd(NO <sub>2</sub> ) <sub>3</sub> [F]	29A-02	•	•	•	•	•			•	•						•	

Subvolume III/36B1		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellanea
No.	Substance																	
30 KNO <sub>3</sub> family																		
30A Pure compounds																		
1	NaNO <sub>3</sub> [F]	30A-01	•	•	•	•	•	•		•	•	•			•	•		
2	KNO <sub>3</sub> [F]	30A-02	•	•	•	•	•	•		•	•	•	•		•	•	•	•
3	RbNO <sub>3</sub> [(A)]	30A-03	•	•	•	•	•	•			•	•	•			•		
4	CsNO <sub>3</sub>	30A-04	•	•	•		•	•	•	•	•	•	•					
30B Solid solutions																		
1	KNO <sub>3</sub> –NH <sub>4</sub> NO <sub>3</sub>	30B-01	•		•		•					•						
2	KNO <sub>3</sub> –RbNO <sub>3</sub>	30B-02	•		•	•	•											
3	KNO <sub>3</sub> –KNO <sub>2</sub>	30B-03	•		•													
4	KNO <sub>3</sub> –KI	30B-04					•											
5	RbNO <sub>3</sub> –CsNO <sub>3</sub>	30B-05	•		•	•	•											
31 LiH <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub> family																		
31A Pure compounds																		
1	LiH <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub> [F]	31A-01	•	•	•	•	•		•	•	•	•	•		•		•	
2	NaH <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub> [F]	31A-02	•	•	•	•	•	•	•	•	•	•	•		•	•	•	
3	KH <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub>	31A-03	•	•	•	•	•	•		•	•	•			•			
4	RbH <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub> [F]	31A-04	•	•	•	•	•			•	•	•			•	•	•	
5	CsH <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub> [(A)]	31A-05	•	•	•	•	•	•		•	•				•			
6	TlH <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub> [F]	31A-06	•		•		•			•								
7	NH <sub>4</sub> H <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub>	31A-07	•	•	•		•				•				•			
32 KIO <sub>3</sub> family																		
32A Pure compounds																		
1	KIO <sub>3</sub> [F]	32A-01	•	•	•	•	•	•	•	•	•	•	•		•			•
2	NH <sub>4</sub> IO <sub>3</sub> [F]	32A-02	•	•	•	•	•	•	•	•	•	•			•		•	
3	KIO <sub>3</sub> ·HIO <sub>3</sub> [(F)]	32A-03	•	•	•		•	•			•				•			

Subvolume III/36B1		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellaneous
No.	Substance																	
33 KDP (KH <sub>2</sub> PO <sub>4</sub> ) family																		
33A Pure compounds																		
1	KH <sub>2</sub> PO <sub>4</sub> [F]	33A-01	•	•	•	•	•	•	•	•	•	•	•		•	•	•	•
2	RbH <sub>2</sub> PO <sub>4</sub> [F]	33A-02	•	•	•	•	•	•	•	•	•	•	•		•	•	•	•
3	CsH <sub>2</sub> PO <sub>4</sub> [F]	33A-03	•	•	•	•	•	•	•	•	•	•	•		•	•	•	
4	TiH <sub>2</sub> PO <sub>4</sub> [D: A]	33A-04	•	•	•		•	•		•		•			•	•	•	
5	NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub> [(A)]	33A-05	•	•	•	•	•	•	•	•	•	•	•		•	•		•
6	(CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> H <sub>2</sub> PO <sub>4</sub> [F]	33A-06	•	•	•		•											
7	KH <sub>2</sub> AsO <sub>4</sub> [F]	33A-07	•	•	•	•	•	•	•	•	•	•	•		•		•	
8	RbH <sub>2</sub> AsO <sub>4</sub> [F]	33A-08	•		•	•	•		•	•	•	•	•		•			•
9	CsH <sub>2</sub> AsO <sub>4</sub> [F]	33A-09	•	•	•	•	•	•	•	•	•	•	•		•	•		
10	TiH <sub>2</sub> AsO <sub>4</sub> [(A)]	33A-10	•	•	•		•				•	•	•		•			•
11	NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub> [(A)]	33A-11	•	•	•	•	•	•	•	•	•	•	•		•			
12	(CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> H <sub>2</sub> AsO <sub>4</sub> [F]	33A-12	•	•	•		•											
33B Solid solutions																		
1	KH <sub>2</sub> PO <sub>4</sub> –NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub>	33B-01	•		•	•	•	•			•	•	•					•
2	KH <sub>2</sub> PO <sub>4</sub> –KH <sub>2</sub> AsO <sub>4</sub>	33B-02	•				•	•							•		•	
3	RbH <sub>2</sub> PO <sub>4</sub> –CsH <sub>2</sub> PO <sub>4</sub>	33B-03	•				•											
4	RbH <sub>2</sub> PO <sub>4</sub> –TiH <sub>2</sub> PO <sub>4</sub>	33B-04	•												•			
5	RbH <sub>2</sub> PO <sub>4</sub> –NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub> (RADP)	33B-05	•		•	•	•	•		•	•	•			•	•		
6	CsH <sub>2</sub> PO <sub>4</sub> –TiH <sub>2</sub> PO <sub>4</sub>	33B-06	•		•		•											
7	TiH <sub>2</sub> PO <sub>4</sub> –NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub>	33B-07	•		•		•		•	•								
8	NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub> –NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub>	33B-08	•															
9	KH <sub>2</sub> AsO <sub>4</sub> –NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub>	33B-09	•				•											
10	RbH <sub>2</sub> AsO <sub>4</sub> –NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub> (RADA)	33B-10	•				•				•	•			•			
11	CsH <sub>2</sub> AsO <sub>4</sub> –NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub>	33B-11	•				•											
12	TiH <sub>2</sub> AsO <sub>4</sub> –NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub>	33B-12	•		•	•	•											
13	Rb <sub>1–x</sub> (NH <sub>4</sub> ) <sub>x</sub> H <sub>2</sub> P <sub>1–y</sub> As <sub>y</sub> O <sub>4</sub> (RADPA)	33B-13	•				•											

Subvolume III/36B1		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellanea
No.	Substance																	
34 PbHPO <sub>4</sub> family																		
34A Pure compounds																		
1	PbHPO <sub>4</sub> [F]	34A-01	•	•	•	•	•	•		•	•	•		•	•	•	•	
2	PbHAsO <sub>4</sub> [F]	34A-02	•	•	•		•				•	•			•			
35 KTiOPO <sub>4</sub> (KTP) family																		
35A Pure compounds																		
1	NaSbOSiO <sub>4</sub> [(F)]	35A-01	•	•	•	•		•			•		•					
2	KSbOSiO <sub>4</sub> [(F)]	35A-02	•	•	•	•	•	•			•		•					
3	AgSbOSiO <sub>4</sub> [(F)]	35A-03	•	•	•						•							
4	NH <sub>4</sub> TiOPO <sub>4</sub>	35A-04	•	•	•						•							•
5	NaTiOPO <sub>4</sub>	35A-05	•												•			
6	KTiOPO <sub>4</sub> [F]	35A-06	•	•	•	•	•	•	•	•	•	•	•		•		•	•
7	KVOPO <sub>4</sub>	35A-07	•	•	•						•			•				
8	KGeOPO <sub>4</sub>	35A-08	•	•	•	•	•			•	•							
9	RbTiOPO <sub>4</sub> [(F)]	35A-09	•	•	•		•		•	•	•	•	•		•		•	•
10	AgTiOPO <sub>4</sub>	35A-10	•	•	•						•							
11	KSnOPO <sub>4</sub> [(F)]	35A-11	•	•	•		•				•		•					
12	RbSnOPO <sub>4</sub>	35A-12	•	•							•							
13	TiTiOPO <sub>4</sub> [(F)]	35A-13	•	•	•		•			•	•	•						
14	NaSbOGeO <sub>4</sub>	35A-14	•	•	•						•							
15	KSbOGeO <sub>4</sub> [(F)]	35A-15	•	•	•	•	•	•			•							
16	RbSbOGeO <sub>4</sub> [(F)]	35A-16	•	•	•		•	•			•		•					
17	KTaOGeO <sub>4</sub> [(F)]	35A-17	•	•	•		•				•							
18	AgSbOGeO <sub>4</sub> [(F)]	35A-18	•	•	•						•							
19	TlSbOGeO <sub>4</sub> [(F)]	35A-19	•	•	•	•					•							
20	KTiOAsO <sub>4</sub> [(F)]	35A-20	•	•	•	•	•				•	•	•					•
21	RbTiOAsO <sub>4</sub> [(F)]	35A-21	•	•	•						•		•					
22	CsTiOAsO <sub>4</sub> [F]	35A-22	•	•	•		•		•		•		•					
23	TiTiOAsO <sub>4</sub>	35A-23	•	•	•						•							

Subvolume III/36B1		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellanea
No.	Substance																	
35B Solid solutions																		
1	(A,B)(C,D)OPO <sub>4</sub> (A, B = H, NH <sub>4</sub> , Na, K, Rb, Ag, Cs, Tl; C, D = Ti, V, Nb)	35B-01	•	•	•	•	•		•	•	•		•		•			•
2	(A,B)TiOAsO <sub>4</sub> (A, B = K, Rb, Cs)	35B-02			•							•						
3	K(A,B)OGeO <sub>4</sub> (A, B = Ti, Nb, Sb, Ta)	35B-03	•		•						•							
4	K(A,B)O(M,M')O <sub>4</sub> (A, B = Ti, Nb, Sb, Ta; M, M' = P, Si, Ge, As)	35B-04	•	•	•						•		•					•
5	KGaPO <sub>4</sub> F <sub>1-x</sub> (OH) <sub>x</sub>	35B-05	•	•	•						•							
36 CsCoPO <sub>4</sub> family																		
36A Pure compounds																		
1	CsCoPO <sub>4</sub> [F]	36A-01	•	•	•		•											
2	NaSrPO <sub>4</sub> [F]	36A-02	•	•			•											
3	NaCdPO <sub>4</sub> [F]	36A-03	•	•			•											
4	NaPbPO <sub>4</sub> [F]	36A-04	•	•			•											
5	TlBePO <sub>4</sub> [(F)]	36A-05	•		•	•	•	•										
37 NaTh <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> family																		
37A Pure compounds																		
1	NaTh <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> [F]	37A-01	•	•	•	•	•		•		•		•					
2	NaU <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> [F]	37A-02	•	•	•		•											
37B Solid solutions																		
1	NaTh <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> –NaTh <sub>2</sub> (AsO <sub>4</sub> ) <sub>3</sub>	37B-01					•											
2	NaTh <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> –NaCe <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub>	37B-02					•											
38 Te(OH) <sub>6</sub> ·2NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub> ·(NH <sub>4</sub> ) <sub>2</sub> HPO <sub>4</sub>																		
38A Pure compound																		
1	Te(OH) <sub>6</sub> ·2NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub> ·(NH <sub>4</sub> ) <sub>2</sub> HPO <sub>4</sub> [F]	38A-01	•	•	•	•	•	•		•	•	•	•		•		•	•



Subvolume III/36B2		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellaneous
No.	Substance																	
39 (NH4)2SO4 family																		
39A Pure compounds																		
1	(NH4)2SO4 [F]	39A-01	•	•	•	•	•	•	•	•	•	•	•		•	•	•	•
2	K2SeO4 [F]	39A-02	•	•	•	•	•	•		•	•	•			•	•		
3	(NH4)2BeF4 [F]	39A-03	•	•	•	•	•	•	•	•	•	•			•	•	•	•
4	[N(CH3)4]2MnCl4	39A-04	•	•	•	•	•	•		•	•					•		
5	[N(CH3)4]2FeCl4 [F]	39A-05	•	•	•	•	•	•		•						•		•
6	K2CoCl4 [F]	39A-06	•	•	•	•	•	•								•		
7	Rb2CoCl4 [F]	39A-07	•	•	•		•	•		•		•				•		
8	[N(CH3)4]2CoCl4 [F]	39A-08	•	•	•		•	•		•	•	•			•	•		
9	K2ZnCl4 [F]	39A-09	•	•	•	•	•	•	•	•	•	•	•		•	•	•	
10	Rb2ZnCl4 [F]	39A-10	•	•	•	•	•	•		•	•	•	•		•	•	•	•
11	(NH4)2ZnCl4 [F]	39A-11	•	•	•	•	•			•	•	•			•	•		•
12	[N(CH3)4]2ZnCl4 [F]	39A-12	•	•	•	•	•	•		•	•	•			•	•	•	•
13	K2CoBr4 [F]	39A-13	•	•	•		•									•		
14	Rb2CoBr4 [F, (A)]	39A-14	•	•	•		•									•		
15	[N(CH3)4]2CuBr4 [F]	39A-15	•	•	•	•	•	•			•					•		
16	K2ZnBr4 [F]	39A-16	•	•	•		•	•								•		
17	Rb2ZnBr4 [F, (A)]	39A-17	•	•	•	•	•	•		•	•	•	•		•	•		•
18	(NH4)2ZnBr4 [F]	39A-18	•	•	•		•				•	•			•	•		
19	K2CoI4 [F]	39A-19	•	•	•		•											
20	K2ZnI4 [F]	39A-20	•	•	•		•											
21	Tl2ZnI4 [F]	39A-21	•	•	•		•					•	•					
22	[N(CH3)4]2ZnI4 [F]	39A-22	•	•	•		•	•			•	•			•			
39B Solid solutions																		
1	(NH4)2SO4–K2SO4	39B-01	•	•	•		•				•				•			
2	(NH4)2SO4–Rb2SO4	39B-02	•	•	•		•				•	•			•			
3	(NH4)2SO4–Cs2SO4	39B-03	•	•	•		•								•			
4	(NH4)2SO4–(NH4)2BeF4	39B-04	•		•	•		•							•	•		
5	[N(CH3)4]2MnCl4–[N(CH3)4]2ZnCl4	39B-05	•															

Subvolume III/36B2		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellanea
No.	Substance																	
6	$[\text{N}(\text{CH}_3)_4]_2\text{CoCl}_4\text{--}[\text{N}(\text{CH}_3)_4]_2\text{ZnCl}_4$	39B-06	•															
7	$\text{K}_2\text{ZnCl}_4\text{--Rb}_2\text{ZnCl}_4$	39B-07	•				•									•	•	
8	$\text{Rb}_2\text{ZnCl}_4\text{--Cs}_2\text{ZnCl}_4$	39B-08					•											
9	$(\text{NH}_4)_2\text{ZnCl}_4\text{--}(\text{NH}_4)_2\text{ZnBr}_4$	39B-09	•	•												•		
10	$[\text{N}(\text{CH}_3)_4]_2\text{ZnCl}_4\text{--}[\text{N}(\text{CH}_3)_4]_2\text{ZnBr}_4$	39B-10	•		•		•					•				•		
11	$[\text{N}(\text{CH}_3)_4]_2\text{CuBr}_4\text{--}[\text{N}(\text{CH}_3)_4]_2\text{CuCl}_4$	39B-11	•				•									•		
<b>40 <math>\text{NH}_4\text{HSO}_4</math> family</b>																		
<b>40A Pure compounds</b>																		
1	$\text{KHSO}_4$	40A-01													•			
2	$\text{RbHSO}_4 [\text{F}]$	40A-02	•	•	•		•	•		•	•	•			•		•	
3	$\text{CsHSO}_4$	40A-03	•	•	•					•					•			
4	$\text{TiHSO}_4$	40A-04													•			
5	$\text{NH}_4\text{HSO}_4 [\text{F}]$	40A-05	•	•	•		•	•			•	•	•		•	•	•	
6	$\text{N}(\text{CH}_3)_4\text{HSO}_4 [(\text{F})]$	40A-06	•	•	•		•	•			•					•		
7	$\text{RbHSeO}_4 [\text{F}]$	40A-07	•	•	•	•	•				•	•			•		•	
8	$\text{CsHSeO}_4$	40A-08	•	•	•										•			
9	$\text{NH}_4\text{HSeO}_4 [\text{F}]$	40A-09	•	•	•	•	•	•		•	•	•			•	•	•	•
<b>40B Solid solutions</b>																		
1	$\text{RbHSO}_4\text{--CsHSO}_4$	40B-01			•													
2	$\text{RbHSO}_4\text{--RbHSeO}_4$	40B-02	•				•											
3	$\text{CsHSO}_4\text{--NH}_4\text{HSO}_4$	40B-03	•		•													
4	$\text{NH}_4\text{HSO}_4\text{--NH}_4\text{HSeO}_4$	40B-04	•				•											
5	$\text{RbHSeO}_4\text{--NH}_4\text{HSeO}_4$	40B-05	•				•											
<b>41 <math>\text{NH}_4\text{LiSO}_4</math> family</b>																		
<b>41A Pure compounds</b>																		
1	$\text{NaLiSO}_4$	41A-01			•										•			
2	$\text{KLiSO}_4$	41A-02	•	•	•	•	•	•	•	•	•	•			•	•	•	

Subvolume III/36B2		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellanea
No.	Substance																	
3	RbLiSO <sub>4</sub> [F]	41A-03	•	•	•		•	•			•	•	•			•		
4	CsLiSO <sub>4</sub>	41A-04	•	•	•					•	•	•			•	•		
5	NH <sub>4</sub> LiSO <sub>4</sub> [F]	41A-05	•	•	•	•	•	•		•	•	•			•	•	•	•
6	CsRbSeO <sub>4</sub> [F]	41A-06	•		•		•	•										•
7	RbLiMoO <sub>4</sub> [F]	41A-07	•		•													•
8	CsLiMoO <sub>4</sub> [F]	41A-08	•	•	•		•			•	•				•			
9	CsLiWO <sub>4</sub> [F]	41A-09	•		•		•	•			•							
<b>41B Solid solutions</b>																		
1	RbLiSO <sub>4</sub> –CsLiSO <sub>4</sub>	41B-01	•													•		
2	RbLiSO <sub>4</sub> –NH <sub>4</sub> LiSO <sub>4</sub>	41B-02	•													•		
<b>42 (NH<sub>4</sub>)<sub>3</sub>H(SO<sub>4</sub>)<sub>2</sub> family</b>																		
<b>42A Pure compounds</b>																		
1	(NH <sub>4</sub> ) <sub>3</sub> H(SO <sub>4</sub> ) <sub>2</sub> [F]	42A-01	•	•	•	•	•	•			•	•	•		•			
2	(NH <sub>4</sub> ) <sub>3</sub> H(SeO <sub>4</sub> ) <sub>2</sub> [F]	42A-02	•	•	•	•	•	•		•	•	•	•		•			•
<b>43 Langbeinite (K<sub>2</sub>Mg<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>) family</b>																		
<b>43A Pure compounds</b>																		
1	(NH <sub>4</sub> ) <sub>2</sub> Mg <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	43A-01	•		•	•	•	•							•			
2	K <sub>2</sub> Mg <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	43A-02	•	•	•		•	•			•		•		•			
3	Rb <sub>2</sub> Mg <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	43A-03			•		•								•			
4	K <sub>2</sub> Ca <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	43A-04	•		•			•			•		•		•			
5	Rb <sub>2</sub> Ca <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	43A-05	•		•		•								•			
6	(NH <sub>4</sub> ) <sub>2</sub> Ca <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	43A-06	•		•		•											
7	(NH <sub>4</sub> ) <sub>2</sub> Mn <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	43A-07	•	•	•						•				•			
8	K <sub>2</sub> Mn <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	43A-08	•	•	•	•	•	•		•	•	•		•	•			
9	K <sub>2</sub> Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	43A-09	•		•		•								•			
10	K <sub>2</sub> Co <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> [(F)]	43A-10	•	•	•		•	•			•	•		•				

Subvolume III/36B2		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellanea
No.	Substance																	
11	$\text{K}_2\text{Zn}_2(\text{SO}_4)_3$ [(F)]	43A-11	•	•	•		•			•					•		•	
12	$\text{K}_2\text{Cd}_2(\text{SO}_4)_3$	43A-12	•	•	•	•	•	•	•	•	•	•	•		•	•	•	
13	$(\text{NH}_4)_2\text{Cd}_2(\text{SO}_4)_3$ [F]	43A-13	•	•	•	•	•	•	•	•	•	•			•		•	
14	$\text{Rb}_2\text{Cd}_2(\text{SO}_4)_3$ [F]	43A-14	•	•	•	•	•	•		•	•	•			•		•	
15	$\text{Tl}_2\text{Cd}_2(\text{SO}_4)_3$ [F]	43A-15	•	•	•	•	•	•		•	•	•			•		•	
16	$\text{K}_2\text{Mn}_2(\text{BeF}_4)_3$	43A-16	•	•	•													
<b>43B Solid solutions</b>																		
1	$\text{Tl}_2\text{Cd}_2(\text{SO}_4)_3-(\text{NH}_4)_2\text{Cd}_2(\text{SO}_4)_3$	43B-01	•	•	•		•			•								
2	$(\text{NH}_4)_2\text{Mn}_2(\text{SO}_4)_3-(\text{NH}_4)_2\text{Cd}_2(\text{SO}_4)_3$	43B-02			•													
3	$\text{Tl}_2\text{Cd}_2(\text{SO}_4)_3-\text{K}_2\text{Cd}_2(\text{SO}_4)_3$	43B-03	•		•													
4	$(\text{NH}_4)_2\text{Mn}_2(\text{SO}_4)_3-\text{K}_2\text{Mn}_2(\text{SO}_4)_3$	43B-04		•	•			•										
5	$\text{K}_2\text{Mn}_2(\text{SO}_4)_3-\text{Tl}_2\text{Mn}_2(\text{SO}_4)_3$	43B-05	•	•	•			•										
6	$(\text{NH}_4)_2\text{Mn}_2(\text{SO}_4)_3-(\text{NH}_4)_2\text{Mn}_2(\text{SeO}_4)_3$	43B-06	•	•	•			•										
7	$\text{Tl}_2\text{Mn}_2(\text{SO}_4)_3-\text{Tl}_2\text{Mn}_2(\text{SeO}_4)_3$	43B-07	•	•														
8	$\text{K}_2\text{Mn}_2(\text{SO}_4)_3-\text{K}_2\text{Mn}_2(\text{SeO}_4)_3$	43B-08	•	•	•													
<b>44 <math>\text{NaNH}_4\text{SO}_4 \cdot 2\text{H}_2\text{O}</math> (lecontite) family</b>																		
<b>44A Pure compounds</b>																		
1	$\text{NaNH}_4\text{SO}_4 \cdot 2\text{H}_2\text{O}$ [F]	44A-01	•	•	•	•	•	•			•	•			•		•	
2	$\text{NaNH}_4\text{SeO}_4 \cdot 2\text{H}_2\text{O}$ [F]	44A-02	•	•	•		•	•	•	•	•	•			•			
<b>44B Solid solution</b>																		
1	$\text{NaNH}_4\text{SO}_4 \cdot 2\text{H}_2\text{O}-\text{NaNH}_4\text{SeO}_4 \cdot 2\text{H}_2\text{O}$	44B-01	•				•											
<b>45 <math>(\text{NH}_4)_2\text{Fe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}</math> family</b>																		
<b>45A Pure compounds</b>																		
1	$\text{NH}_4\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-01	•	•	•		•											
2	$\text{NH}_4\text{V}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-02	•	•	•		•											
3	$\text{NH}_4\text{Cr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-03	•	•	•		•											

Subvolume III/36B2		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellanea
No.	Substance																	
4	$\text{NH}_4\text{Fe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-04	•	•	•		•				•				•			
5	$\text{NH}_4\text{In}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-05	•	•	•		•											
6	$\text{CH}_3\text{NH}_3\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-06	•	•	•	•	•			•	•				•			
7	$\text{CH}_3\text{NH}_3\text{V}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-07	•	•	•		•											
8	$\text{CH}_3\text{NH}_3\text{Cr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-08	•	•	•		•	•							•			
9	$\text{CH}_3\text{NH}_3\text{Fe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-09	•	•	•		•				•							
10	$\text{CH}_3\text{NH}_3\text{Ga}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-10	•	•			•				•				•			
11	$\text{CH}_3\text{NH}_3\text{In}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-11	•	•	•		•											
12	$\text{CH}_3\text{NH}_3\text{Al}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-12	•	•	•		•				•				•			
13	$\text{CH}_3\text{NH}_3\text{Cr}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-13	•		•		•											
14	$\text{CH}_3\text{NH}_3\text{Ga}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-14	•		•		•											
15	$\text{N}_2\text{H}_5\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ [F]	45A-15	•	•	•		•											
16	$\text{CO}(\text{NH}_2)_2\text{HCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	45A-16	•															
<b>45B Solid solutions</b>																		
1	$\text{CH}_3\text{NH}_3\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O} - \text{NH}_2\text{NH}_3\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	45B-01	•				•											
2	$\text{CH}_3\text{NH}_3\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O} - \text{CH}_3\text{NH}_3\text{Al}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$	45B-02	•				•											
<b>46 GASH (<math>\text{C}(\text{NH}_2)_3\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}</math>) family</b>																		
<b>46A Pure compounds</b>																		
1	$\text{C}(\text{NH}_2)_3\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ [F]	46A-01	•	•	•	•	•		•	•	•	•	•		•		•	•
2	$\text{C}(\text{NH}_2)_3\text{V}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ [F]	46A-02	•		•		•							•	•			
3	$\text{C}(\text{NH}_2)_3\text{Cr}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ [F]	46A-03	•		•		•								•			
4	$\text{C}(\text{NH}_2)_3\text{Ga}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ [F]	46A-04	•	•	•	•	•			•	•				•			
5	$\text{C}(\text{NH}_2)_3\text{Al}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$ [F]	46A-05	•	•	•	•	•			•	•				•			
6	$\text{C}(\text{NH}_2)_3\text{Cr}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$ [F]	46A-06	•		•		•											
7	$\text{C}(\text{NH}_2)_3\text{Ga}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$ [F]	46A-07	•	•	•	•	•			•	•				•		•	
8	$(\text{CH}_3)_2\text{NH}_2\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ [F]	46A-08	•	•	•		•				•	•						•
9	$(\text{CH}_3)_2\text{NH}_2\text{Ga}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ [F]	46A-09	•	•	•	•	•											

Subvolume III/36B2		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellanea
No.	Substance																	
46B Solid solution																		
1	(CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> Al(SO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O– (CH <sub>3</sub> ) <sub>2</sub> NH <sub>2</sub> Al(SeO <sub>4</sub> ) <sub>2</sub> ·6H <sub>2</sub> O	46B-01	•		•													
47 Colemanite (Ca <sub>2</sub> B <sub>6</sub> O <sub>11</sub> ·5H <sub>2</sub> O)																		
47A Pure compound																		
1	Ca <sub>2</sub> B <sub>6</sub> O <sub>11</sub> ·5H <sub>2</sub> O [F]	47A-01	•	•	•		•									•	•	
48 K <sub>4</sub> Fe(CN) <sub>6</sub> ·3H <sub>2</sub> O family																		
48A Pure compounds																		
1	K <sub>4</sub> Mn(CN) <sub>6</sub> ·3H <sub>2</sub> O [F]	48A-01	•				•											
2	K <sub>4</sub> Fe(CN) <sub>6</sub> ·3H <sub>2</sub> O [F]	48A-02	•	•	•		•	•		•	•	•	•		•	•	•	
3	K <sub>4</sub> Ru(CN) <sub>6</sub> ·3H <sub>2</sub> O [F]	48A-03	•		•		•				•				•			
4	K <sub>4</sub> Os(CN) <sub>6</sub> ·3H <sub>2</sub> O [F]	48A-04	•		•		•											
48B Solid solutions																		
1	K <sub>4</sub> Fe(CN) <sub>6</sub> ·3H <sub>2</sub> O–Rb <sub>4</sub> Fe(CN) <sub>6</sub> ·3H <sub>2</sub> O	48B-01	•				•											
2	K <sub>4</sub> Fe(CN) <sub>6</sub> ·3H <sub>2</sub> O–Tl <sub>4</sub> Fe(CN) <sub>6</sub> ·3H <sub>2</sub> O	48B-02	•				•											
3	K <sub>4</sub> Fe(CN) <sub>6</sub> ·3H <sub>2</sub> O– (NH <sub>4</sub> ) <sub>4</sub> Fe(CN) <sub>6</sub> ·3H <sub>2</sub> O	48B-03	•				•											
49 K <sub>3</sub> BiCl <sub>6</sub> ·2KCl·KH <sub>3</sub> F <sub>4</sub>																		
49A Pure compound																		
1	K <sub>3</sub> BiCl <sub>6</sub> ·2KCl·KH <sub>3</sub> F <sub>4</sub> [F]	49A-01	•		•		•			•								

Subvolume III/36B2		No.	Fundamentals	Material preparation	Crystal structure	Lattice distortion	Dielectric properties	Thermal properties	Electromechanical	Elastic properties	Optical properties	Light scattering	Conduction	Magnetism	NMR, ESR	Local structures	Domains	Miscellanea
No.	Substance																	
M Miscellaneous crystals																		
M15 SnTe group																		
M15-i	GeTe [(F)]	M15-i	•	•	•	•	•	•			•	•	•		•		•	
M15-ii	SnTe [(F)]	M15-ii	•	•	•	•	•	•		•	•	•	•		•	•		
M15-iii	Ge <sub>1-x</sub> Sn <sub>x</sub> Te	M15-iii	•	•	•	•		•		•					•			
M15-iv	Pb <sub>1-x</sub> Ge <sub>x</sub> Te	M15-iv	•		•	•	•	•		•	•	•	•			•		
M15-v	Pb <sub>1-x</sub> Sn <sub>x</sub> Te	M15-v	•				•			•	•		•		•			
M15-vi	Cd <sub>1-x</sub> Zn <sub>x</sub> Te	M15-vi	•	•	•		•	•			•	•	•			•		
M16	PbN <sub>6</sub>	M16	•	•		•	•		•								•	•
M17	Sb <sub>2</sub> S <sub>3</sub> [F]	M17	•	•	•		•			•	•		•		•	•	•	
M18	Sb <sub>5</sub> O <sub>7</sub> I [F]	M18	•	•	•	•	•			•	•	•						
M19	H <sub>2</sub> O [(F)]	M19	•		•	•	•	•		•	•	•	•		•	•		
M20 KOH group																		
M20-i	NaOD [(A)]	M20-i	•		•	•	•	•			•	•			•	•		
M20-ii	KOH [(A)]	M20-ii	•		•	•	•	•							•			
M20-iii	RbOH [(F)]	M20-iii	•		•	•		•			•	•			•			
M20-iv	CsOH [(A)]	M20-iv	•		•	•	•	•			•	•			•			
M21	KSCN [(A)]	M21	•	•	•		•	•		•	•	•			•	•		•
M22	Na <sub>3</sub> Sc <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> [(F)]	M22	•	•	•		•				•		•					•
M23	H <sub>2</sub> (UO <sub>2</sub> ) <sub>2</sub> (AsO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O [(A,F)]	M23	•		•		•								•		•	
M24 Li(N <sub>2</sub> H <sub>5</sub> )SO <sub>4</sub> group																		
M24-i	Li(N <sub>2</sub> H <sub>5</sub> )SO <sub>4</sub>	M24-i	•	•	•	•	•	•			•	•	•		•	•		
M24-ii	Li(N <sub>2</sub> H <sub>5</sub> )BeF <sub>4</sub>	M24-ii	•	•	•		•				•		•					
M25	N(CH <sub>3</sub> ) <sub>4</sub> HSO <sub>4</sub> ·H <sub>2</sub> O [(F)]	M25	•	•			•	•										
M26 Ag <sub>2</sub> H <sub>3</sub> IO <sub>6</sub> group																		
M26-i	Ag <sub>2</sub> H <sub>3</sub> IO <sub>6</sub> [(A)]	M26-i	•	•	•		•	•			•				•	•		
M26-ii	(NH <sub>4</sub> ) <sub>2</sub> H <sub>3</sub> IO <sub>6</sub> [(A)]	M26-ii	•	•	•		•	•			•	•			•			
M27 TiNbWO <sub>6</sub> ·nH <sub>2</sub> O group																		
M27-i	RbNbWO <sub>6</sub> ·nH <sub>2</sub> O [(F)]	M27-i	•	•	•		•				•		•				•	
M27-ii	TiNbWO <sub>6</sub> ·nH <sub>2</sub> O [(F)]	M27-ii	•	•	•		•				•		•				•	
M28	NH <sub>4</sub> PF <sub>6</sub> ·NH <sub>4</sub> F [(A)]	M28	•		•		•								•			

## IG Outline of all subvolumes of III/36

**Table IG-1. Substance families contained in all subvolumes of III/36.**

Subvolume A1: Perovskite-type oxides and  $\text{LiNbO}_3$  family

1	Perovskite-type oxides [M. Adachi, Y. Akishige, K. Deguchi, T. Ikeda, M. Okuyama, A. Sakai, E. Sawaguchi, T. Takenaka, T. Tsukamoto, T. Yagi]
1A	Simple perovskite-type oxides
1B	Complex perovskite-type oxides
1B-a	$(\text{A}_{1/2}^{1+}\text{A}_{1/2}^{3+})\text{MO}_3$ - type complex perovskite oxides
1B-b	$\text{A}^{2+}(\text{M}_{1/2}^{2+}\text{M}_{1/2}^{6+})\text{O}_3$ - type complex perovskite oxides
1B-c	$\text{A}^{2+}(\text{M}_{1/2}^{3+}\text{M}_{1/2}^{5+})\text{O}_3$ - type complex perovskite oxides
1B-d	$\text{A}^{2+}(\text{M}_{1/3}^{2+}\text{M}_{2/3}^{5+})\text{O}_3$ - type complex perovskite oxides
1B-e	$\text{A}^{2+}(\text{M}_{2/3}^{3+}\text{M}_{1/3}^{6+})\text{O}_3$ - type complex perovskite oxides
1B-f	$\text{A}(\text{M}, \text{M}', \text{M}'')\text{O}_3$ - type complex perovskite oxides
1B-g	$(\text{A}, \text{A}')(\text{M}, \text{M}')\text{O}_3$ - type complex perovskite oxides
1C	Solid solutions with perovskite-type oxides as end members
1C-a	Solid solutions with simple perovskite-type oxides as end members
1C-b	Solid solutions with complex perovskite-type oxides as end members
1C-c	Ternary solid solutions, etc. with perovskite-type oxides as constituents
2	$\text{LiNbO}_3$ family [T. Hikita]
2A	Pure compounds
2B	Solid solutions

Subvolume A2: Oxides other than Perovskite-type and  $\text{LiNbO}_3$  family

3	$\text{YMnO}_3$ family [T. Ikeda]
4	$\text{SrTeO}_3$ family [T. Hikita]
5	Stibiotantalite family [M. Adachi]
6	Tungsten-bronze-type oxides [T. Tsukamoto, T. Ikeda]
7	Pyrochlore-type oxides [Y. Akishige]
8	$\text{Sr}_2\text{Nb}_2\text{O}_7$ family [Y. Akishige]
9	Layer-structure oxides [Y. Akishige]
10	$\text{BaAl}_2\text{O}_4$ -type oxides [Y. Akishige]
11	$\text{LaBGeO}_5$ [Y. Iwata]
12	$\text{LiNaGe}_4\text{O}_9$ -type oxides [Y. Iwata]
13	$\text{Li}_2\text{Ge}_7\text{O}_{15}$ family [Y. Iwata]
14	$\text{Pb}_5\text{Ge}_3\text{O}_{11}$ family [Y. Iwata]
15	$5\text{PbO} \cdot 2\text{P}_2\text{O}_5$ [Y. Iwata]



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16	$\text{Ca}_3(\text{VO}_4)_2$ family [N. Nakatani]
17	$\text{Gd}_2(\text{MoO}_4)_3$ (GMO) family [N. Nakatani]
18	Boracite-type family [T. Hikita]
19	$\text{Rb}_3\text{MoO}_3\text{F}_3$ family [M. Adachi]
M	Miscellaneous crystals
M1	$\text{TiO}_2$ [E. Nakamura]
M2	$\text{WO}_3$ [M. Adachi]
M3	$\text{NaVO}_3$ group [E. Nakamura]
M4	$\text{Fe}_3\text{O}_4$ [Y. Akishige]
M5	$\text{RVO}_4$ (R = Sc, Nd, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) [T. Asahi]
M6	$\text{RAsO}_4$ (R = Pr, Nd, Eu, Gd, Tb, Dy, Er, Yb) [T. Asahi]
M7	$\text{Cr}_2\text{BeO}_4$ [K. Deguchi]
M8	$\text{RMn}_2\text{O}_5$ (R = Y, Eu, Gd, Tb, Dy, Bi) [K. Deguchi]
M9	$\text{Pb}_3\text{TeO}_6$ [M. Adachi]
M10	$\text{Li}_2\text{B}_4\text{O}_7$ [M. Adachi]
M11	$\text{Ag}_{26}\text{I}_{18}\text{W}_4\text{O}_{16}$ [M. Adachi]
M12	$\text{Sr}_8[\text{Al}_{12}\text{O}_{24}](\text{CrO}_4)_2$ [M. Adachi]
M13	$\text{Pb}_5\text{Mo}_3\text{O}_9\text{F}_{10}$ group [K. Deguchi]
M14	$\text{Pb}_5\text{Cr}_3\text{F}_{19}$ group [K. Deguchi]

Subvolume B1: Inorganic substances other than oxides  
SbSI family ... TAAP

20	SbSI family [T. Yagi]
21	TlS [Y. Shiozaki]
22	$\text{TlInS}_2$ family [Y. Shiozaki]
23	$\text{Ag}_3\text{AsS}_3$ family [K. Deguchi]
24	$\text{Sn}_2\text{P}_2\text{S}_6$ family [K. Deguchi]
25	$\text{KNiCl}_3$ family [Y. Shiozaki]
26	$\text{BaMnF}_4$ family [K. Deguchi]
27	HCl family [K. Gesi]
28	$\text{NaNO}_2$ family [K. Gesi]
29	$\text{CsCd}(\text{NO}_2)_3$ family [K. Hasebe, T. Asahi]
30	$\text{KNO}_3$ family [K. Gesi]
31	$\text{LiH}_3(\text{SeO}_3)_2$ family [M. Komukae, T. Osaka]
32	$\text{KIO}_3$ family [K. Hasebe, T. Asahi]
33	KDP ( $\text{KH}_2\text{PO}_4$ ) family [E. Nakamura, M. Komukae, T. Osaka]
34	$\text{PbHPO}_4$ family [K. Gesi]
35	$\text{KTiOPO}_4$ (KTP) family [T. Hikita]
36	$\text{CsCoPO}_4$ family [N. Nakatani]
37	$\text{NaTh}_2(\text{PO}_4)_3$ family [Y. Shiozaki]
38	$\text{Te}(\text{OH})_6 \cdot 2\text{NH}_4\text{H}_2\text{PO}_4 \cdot (\text{NH}_4)_2\text{HPO}_4$ [E. Nakamura]

## Subvolume B2: Inorganic substances other than oxides

(NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> family ... K<sub>3</sub>BiCl<sub>6</sub> · 2KCl · KH<sub>3</sub>F<sub>4</sub>

- 39 (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> family [K. Deguchi, K. Hasebe, K. Gesi, T. Asahi]
- 40 NH<sub>4</sub>HSO<sub>4</sub> family [T. Yagi]
- 41 NH<sub>4</sub>LiSO<sub>4</sub> family [T. Yagi]
- 42 (NH<sub>4</sub>)<sub>3</sub>H(SO<sub>4</sub>)<sub>2</sub> family [K. Gesi]
- 43 Langbeinite-type family [T. Hikita]
- 44 Lecontite (NaNH<sub>4</sub>SO<sub>4</sub>·2H<sub>2</sub>O) family [M. Komukae, T. Osaka]
- 45 Alum family [M. Komukae, T. Osaka]
- 46 GASH (C(NH<sub>2</sub>)<sub>3</sub>Al(SO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O) family [K. Gesi]
- 47 Colemanite (Ca<sub>2</sub>B<sub>6</sub>O<sub>11</sub>·5H<sub>2</sub>O) [M. Komukae, T. Osaka]
- 48 K<sub>4</sub>Fe(CN)<sub>6</sub>·3H<sub>2</sub>O family [M. Komukae, T. Osaka]
- 49 K<sub>3</sub>BiCl<sub>6</sub>·2KCl·KH<sub>3</sub>F<sub>4</sub> [Y. Shiozaki]
- M15 SnTe group [Y. Akishige]
- M16 PbN<sub>6</sub> [E. Nakamura]
- M17 Sb<sub>2</sub>S<sub>3</sub> [T. Yagi]
- M18 Sb<sub>5</sub>O<sub>7</sub>I [T. Yagi]
- M19 H<sub>2</sub>O [N. Nakatani]
- M20 KOH group [E. Nakamura]
- M21 KSCN [E. Nakamura]
- M22 Na<sub>3</sub>Sc<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub> [E. Nakamura]
- M23 H<sub>2</sub>(UO<sub>2</sub>)<sub>2</sub>(AsO<sub>4</sub>)<sub>2</sub>·8H<sub>2</sub>O [E. Nakamura]
- M24 Li(N<sub>2</sub>H<sub>5</sub>)SO<sub>4</sub> group [E. Nakamura]
- M25 N(CH<sub>3</sub>)<sub>4</sub>HSO<sub>4</sub>·H<sub>2</sub>O [E. Nakamura]
- M26 Ag<sub>2</sub>H<sub>3</sub>IO<sub>6</sub> group [E. Nakamura]
- M27 TiNbWO<sub>6</sub>·nH<sub>2</sub>O group [E. Nakamura]
- M28 NH<sub>4</sub>PF<sub>6</sub>·NH<sub>4</sub>F [E. Nakamura]

## Subvolume C: Organic crystals, liquid crystals and polymers

- 50 SC(NH<sub>2</sub>)<sub>2</sub> family [Y. Shiozaki, T. Asahi]
- 51 CCl<sub>3</sub>CONH<sub>2</sub> [Y. Shiozaki]
- 52 Cu(HCOO)<sub>2</sub>·4H<sub>2</sub>O [M. Komukae, T. Osaka]
- 53 N(CH<sub>3</sub>)<sub>4</sub>HgCl<sub>3</sub> family [M. Adachi]
- 54 CH<sub>3</sub>NH<sub>3</sub>AlCl<sub>4</sub> family [Y. Shiozaki]
- 55 [(CH<sub>3</sub>)<sub>2</sub>NH<sub>2</sub>]<sub>2</sub>CoCl<sub>4</sub> family [K. Hasebe, T. Asahi]
- 56 [(CH<sub>3</sub>)<sub>2</sub>NH<sub>2</sub>]<sub>3</sub>Sb<sub>2</sub>Cl<sub>9</sub> family [K. Hasebe, T. Asahi]
- 57 (CH<sub>3</sub>NH<sub>3</sub>)<sub>5</sub>Bi<sub>2</sub>Cl<sub>11</sub> family [K. Hasebe, T. Asahi]
- 58 DSP (Ca<sub>2</sub>Sr(CH<sub>3</sub>CH<sub>2</sub>COO)<sub>6</sub>) family [E. Nakamura]
- 59 (CH<sub>2</sub>ClCOO)<sub>2</sub>H·NH<sub>4</sub> family [E. Nakamura]

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- 60  $(\text{NH}_2\text{CH}_2\text{COOH})_3 \cdot \text{H}_2\text{SO}_4$  (TGS) family [N. Nakatani]  
61  $\text{NH}_2\text{CH}_2\text{COOH} \cdot \text{AgNO}_3$  [E. Nakamura]  
62  $(\text{NH}_2\text{CH}_2\text{COOH})_2 \cdot \text{HNO}_3$  [K. Gesi]  
63  $(\text{NH}_2\text{CH}_2\text{COOH})_2 \cdot \text{MnCl}_2 \cdot 2\text{H}_2\text{O}$  [M. Komukae, T. Osaka]  
64  $(\text{CH}_3\text{NHCH}_2\text{COOH})_3 \cdot \text{CaCl}_2$  [M. Komukae, T. Osaka]  
65  $(\text{CH}_3)_3\text{NCH}_2\text{COO} \cdot \text{H}_3\text{PO}_4$  family [K. Deguchi]  
66  $(\text{CH}_3)_3\text{NCH}_2\text{COO} \cdot \text{CaCl}_2 \cdot 2\text{H}_2\text{O}$  [E. Nakamura]  
67 Rochelle salt  $(\text{NaKC}_4\text{H}_4\text{O}_6 \cdot 4\text{H}_2\text{O})$  family [Y. Shiozaki, E. Nakamura]  
68  $\text{LiNH}_4\text{C}_4\text{H}_4\text{O}_6 \cdot \text{H}_2\text{O}$  family [K. Deguchi]  
69  $\text{C}_5\text{H}_6\text{NBF}_4$  [N. Nakatani]  
70  $3\text{C}_6\text{H}_4(\text{OH})_2 \cdot \text{CH}_3\text{OH}$  [N. Nakatani]  
71 Ferroelectric and antiferroelectric liquid crystals  
[H. Takezoe, Y. Ishibashi, R. Nozaki, E. Nakamura]  
72 Polymer ferroelectrics [T. Furukawa, R. Nozaki]  
M29  $\text{H}_2\text{NCONHNH}_2 \cdot \text{HCl}$  [E. Nakamura]  
M30  $\text{CaC}_4\text{H}_4\text{O}_6 \cdot 4\text{H}_2\text{O}$  [E. Nakamura]  
M31  $\text{C}_9\text{H}_{18}\text{NO}$  [E. Nakamura]  
M32  $\text{C}_4[\text{CH}_2\text{OC}_6\text{H}_3(\text{NO}_2)_2]_2$  [E. Nakamura]

## III References

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