

I Introduction

IA General remarks

The present Volume III/36, which consists of two subvolumes A and B, 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 and B for non-oxides including liquid crystals. 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 1921, 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 1921 to 1993. Number of ferroelectrics families increases from 48 in III/28 to 72 in III/36. Numbers of tables and figures increase from 395 and 2430 in III/16a and III/28a (supplement to III/16a) to 536 and 3411 in III/36A, respectively.

Printed version and the 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 in 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 CD-ROM. About 6% of tables and 28% of figures in CD-ROM are selected and presented in the printed version. Captions of the tables and figures which appear only in 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.

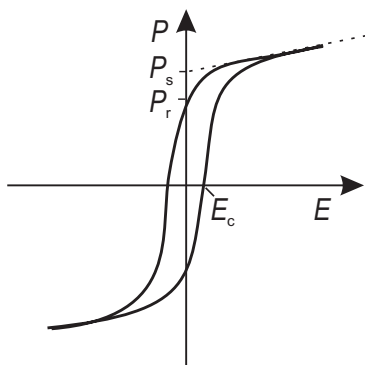


Fig. IB-1. Ferroelectric hysteresis loop. P_s : spontaneous polarization (see remarks on P_s in IC). P_r : remanent polarization. E_c : coercive field.

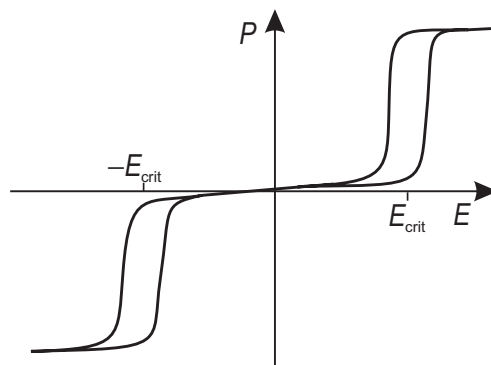


Fig. IB-2. Antiferroelectric hysteresis loop. E_{crit} : critical field.

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 high polymers

In the last two decades active studies have been made on ferroelectric liquid crystals and high polymers, after ferroelectricity was 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 transducer, 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, 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 Chapter 71 in the Subvolume III/36B2. Readers may consult [91Goo], [91Tay], [93Buk], [94Bli], [94Fuk], [98Bli]

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

Ferroelectric high 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]. 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 volume ratio of the crystal regions per total is relatively large (e.g., more than 50 %). Coercive field is larger (e.g., $> 50 \text{ MV/m}$) 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 high polymer ferroelectrics are presented in Chapter 72 in the Subvolume III/36B2.

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 ± 0.012 and 127.3(21) for 127.3 ± 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}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. $\text{P}2_1\text{-C}_2^2$). 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 Θ_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 Θ 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} , β_{ij} , and U_{ij} are called temperature parameters.

The isotropic temperature parameter (sometimes called Debye parameter) B is defined by:

$$= \exp(-B \sin^2 \theta / \lambda^2). \quad (e)$$

In a few publications the mean square displacement of the atom, $u^2 = B/(8\pi^2)$, is listed instead of B .

Discrepancy indices in structure analysis (3)

As a measure of reliability of the result of structure analysis of 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^{th} Bragg reflection, and the summation is extended over all the observable F_i 's.

In powder diffraction studies, 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^{th} Bragg peak. In powder diffraction studies, profile of 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_{prof} is used

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

where y_i is the intensity of scattered X-rays (or neutrons) at the scattering angle 2θ , 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_{nuc} and R_{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 ϵ_{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 ΔD_i , ΔT , and ΔS are changes of the component of electric displacement, temperature and entropy, respectively, and E_j , ρ , c_p and T are 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 ϵ_{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 ϵ_{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 ξ and ζ are given as measures of the dielectric nonlinearity. They should be understood as the values at atmospheric pressure unless otherwise stated. Values of χ_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 κ is the dielectric constant. In general, κ obeys the Curie-Weiss law above the Curie point:

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

where κ_∞ 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 λ , μ , and ν for 1...6. The correspondence between i , j and λ (or μ , ν) 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 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

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

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

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

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

(3) Definitions of various electromechanical coupling factors.

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

The following two coupling factors are used as well:

a) planar coupling factor

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

for a thin disc of piezoelectric ceramics which is poled perpendicular to it (σ^E : Poisson ratio).

b) thickness coupling factor $k_t^2 = e_{33}^2 (\epsilon_{33}^{\mathbf{S}} c_{33}^D)^{-1}$ 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 piezooptic 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) Piezooptic and electrooptic equations

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

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

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

$$P_i(2\nu) = \sum_{j,k} \epsilon_0 d_{ijk} E_j(\nu) E_k(\nu) \quad (f)$$

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 2ν generated by the electric field of light of frequency ν , $E(\nu)$, and ϵ_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 KH_2PO_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
LiIO_3	$d_{31} = -7.1(1.14)$	1.064
LiNbO_3	$d_{31} = -5.95(0.95)$	1.064
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
KH_2PO_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: $\epsilon_0 \leftrightarrow 1/4\pi$. 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 ν_i , ν_s , \mathbf{q}_i , \mathbf{q}_s for ν (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 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 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.

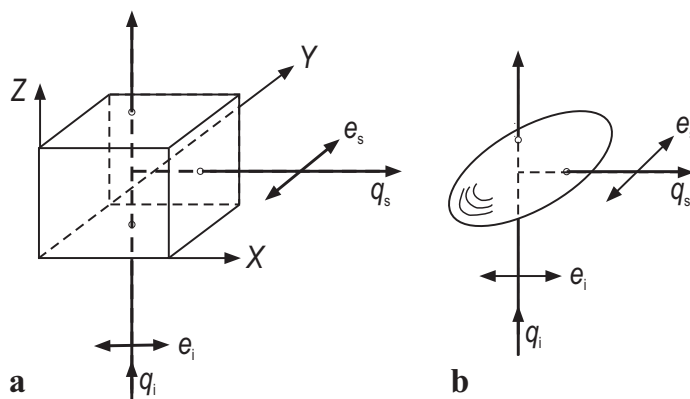


Fig. IC-1. Symbols on scattering geometries. (a) Z(XY)X. (b) HV.

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^{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 ₁	A(X, Y, Z)	
	$\bar{1}$	C _i	A _g	A _u (X, Y, Z)
Monoclinic	2	C ₂	A(Y), B(X, Z)	
	m	C _s	A'(X, Z), A''(Y)	
	2/m	C _{2h}	A _g , B _g	A _u (Y), B _u (X, Z)
Orthorhombic	222	D ₂	A, B ₁ (Z), B ₂ (Y), B ₃ (X)	
	2mm	C _{2v}	A ₁ (Z), A ₂ , B ₁ (X), B ₂ (Y)	
	mmm	D _{2h}	A _g , B _{1g} , B _{2g} , B _{3g}	A _u , B _{1u} (Z), B _{2u} (Y), B _{3u} (X)
Tetragonal	4	C ₄	A(Z), B, E(X, Y)	
	$\bar{4}$	S ₄	A, B(Z), E(X, Y)	
	4/m	C _{4h}	A _g , B _g , E _g	A _u (Z), B _u , E _u (X, Y)
	4mm	C _{4v}	A ₁ (Z), B ₁ , B ₂ , E(X, Y)	A ₂
	422	D ₄	A ₁ , B ₁ , B ₂ , E(X, Y)	A ₂ (Z)
	$\bar{4}2m$	D _{2d}	A ₁ , B ₁ , B ₂ (Z), E(X, Y)	A ₂
	4/mmm	D _{4h}	A _{1g} , B _{1g} , B _{2g} , E _g	A _{2g} , A _{1u} , A _{2u} (Z), B _{1u} , B _{2u} , E _u (X, Y)
Trigonal	3	C ₃	A(Z), E(X, Y)	
	$\bar{3}$	C _{3i}	A _g , E _g	A _u (Z), E _u (X, Y)
	32	D ₃	A ₁ , E(X, Y)	A ₂ (Z)
	3m	C _{3v}	A ₁ (Z), E(X, Y)	A ₂
	$\bar{3}m$	D _{3d}	A _{1g} , E _g	A _{1u} , A _{2u} (Z), E _u (X, Y)
Hexagonal	6	C ₆	A(Z), E ₁ (X, Y), E ₂	B
	$\bar{6}$	3 ₂ h	A', E'(X, Y), E''	A''(Z)
	6/m	C _{6h}	A _g , E _{1g} , E _{2g}	B _g , A _u (Z), E _{1u} (X, Y), E _{2u}
	622	D ₆	A ₁ , E ₁ (X, Y), E ₂	A ₂ (Z), B ₁ , B ₂
	6mm	C _{6v}	A ₁ (Z), E ₁ (X, Y), E ₂	A ₂ , B ₁ , B ₂
	$\bar{6}m2$	D _{3h}	A ₁ ', E'(X, Y), E''	A ₂ ', A ₁ '', A ₂ ''(Z)
	6/mmm	D _{6h}	A _{1g} , E _{1g} , E _{2g}	A _{2g} , B _{1g} , B _{2g} , A _{1u} , A _{2u} (Z), B _{1u} , B _{2u} , E _{1u} (X, Y), E _{2u}
Cubic	23	T	A, E, F(X, Y, Z)	
	m3	T _h	A _g , E _g , F _g	A _u , E _u , F _u (X, Y, Z)
	432	O	A ₁ , E, F ₂	A ₂ , F ₁ (X, Y, Z)
	$\bar{4}3m$	T _d	A ₁ , E, F ₂ (X, Y, Z)	A ₂ , F ₁
	m3m	O _h	A _{1g} , E _g , F _{2g}	A _{2g} , F _{1g} , A _{1u} , A _{2u} , E _u , F _{1u} (X, Y, Z), F _{2u}

*) 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_g and B_{1g} are not. The letters X, Y, Z mean that the mode is infrared active to the incident radiation polarized along the orthogonal 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 μ_0 .

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

The magnetic susceptibility χ_{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 $M/(H(\text{mol}/\text{volume}))$.

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

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

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

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

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

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

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

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

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

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

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

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

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].

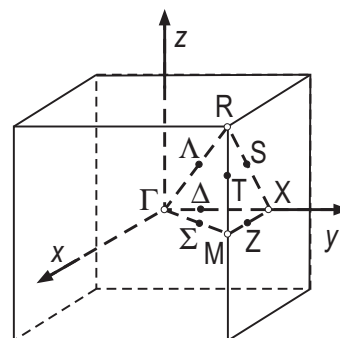


Fig. IC-2. Conventional symbols of special points in reciprocal space (q -space, $q = 2\pi/\lambda$) for the simple cubic lattice. Γ : $\pi/a\{0,0,0\}$, X : $\pi/a\{1,0,0\}$, M : $\pi/a\{1,1,0\}$, R : $\pi/a\{1,1,1\}$. The symbols S , T , Z , Δ , Λ , Σ represent the positions along the lines on which 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° walls. Other ferroelectrics (e.g. 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° 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 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.

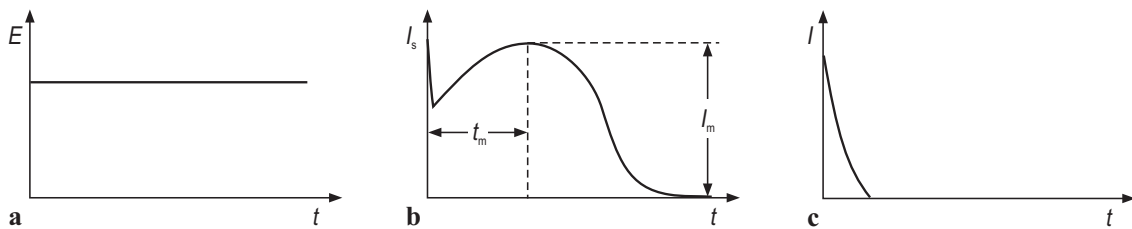


Fig. IC-3. Switching of ferroelectric crystal [67Fat]. E : electric field strength, I : electric current, I_s : switching current, t : time. (a) constant field applied at $t = 0$. (b) switching current I_s obtained with an electric field antiparallel to the original P_s of the crystal. t_s : switching 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 has 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 Figs. ID-1...3.

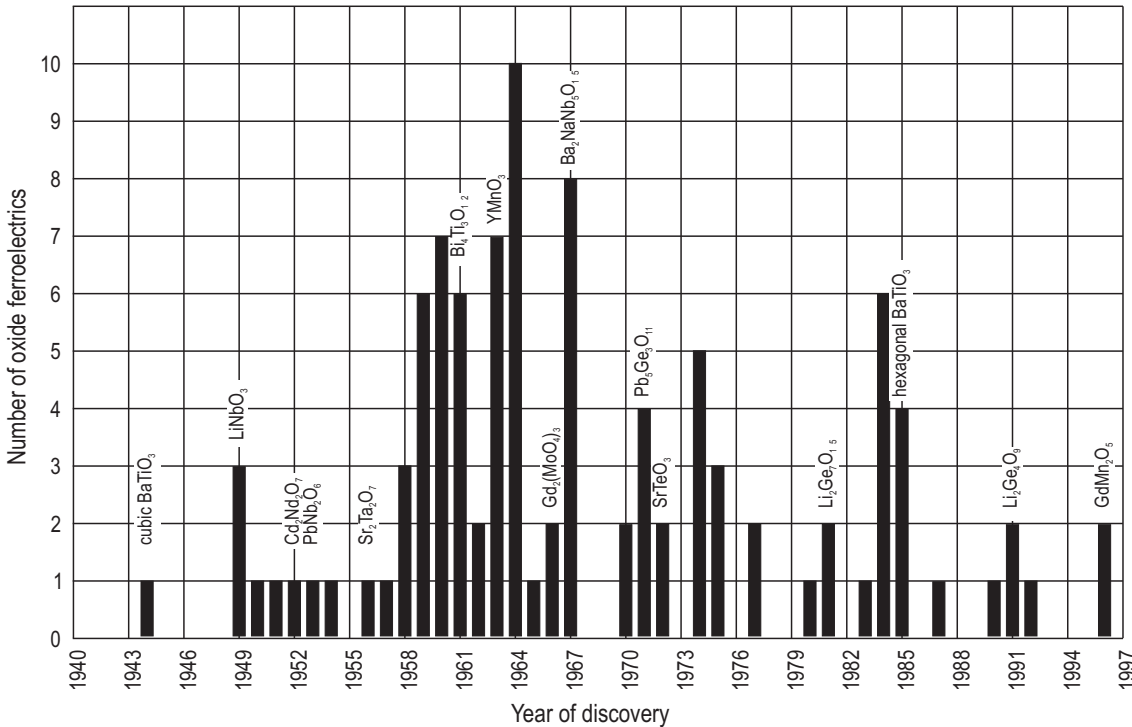


Fig. ID-1. Number of oxide ferroelectrics discovered in each year. Only pure compounds are included. Representatives of the 15 families of oxide ferroelectrics are indicated at the year of discovery. Prepared by K. Deguchi using the information given in subsection 1a of each section.

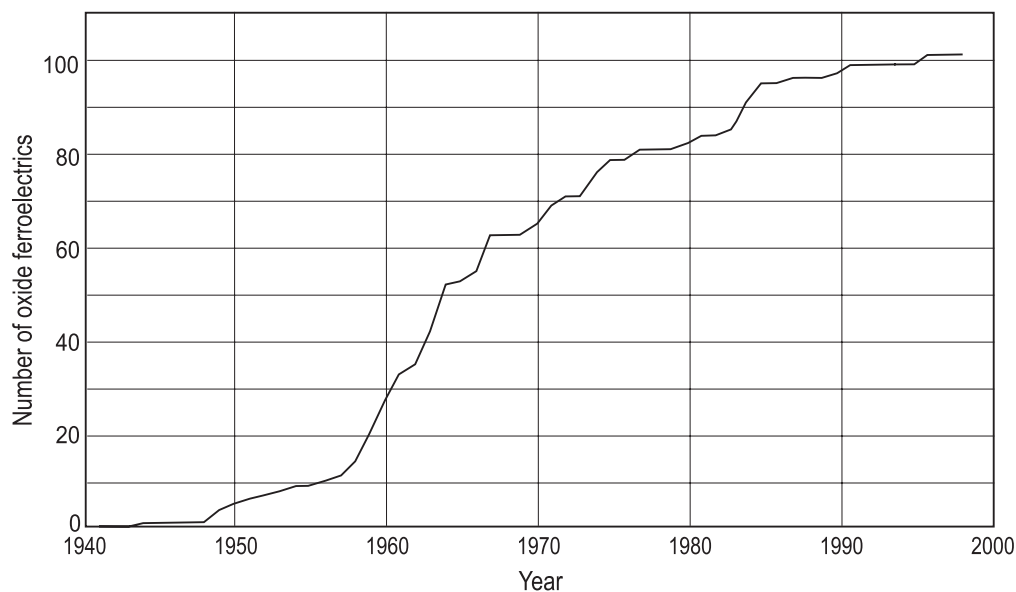


Fig. ID-2. Total number of oxide ferroelectrics known at the end of each year. Only pure compounds are included. Prepared by K. Deguchi using the same information as in Fig. ID-1.

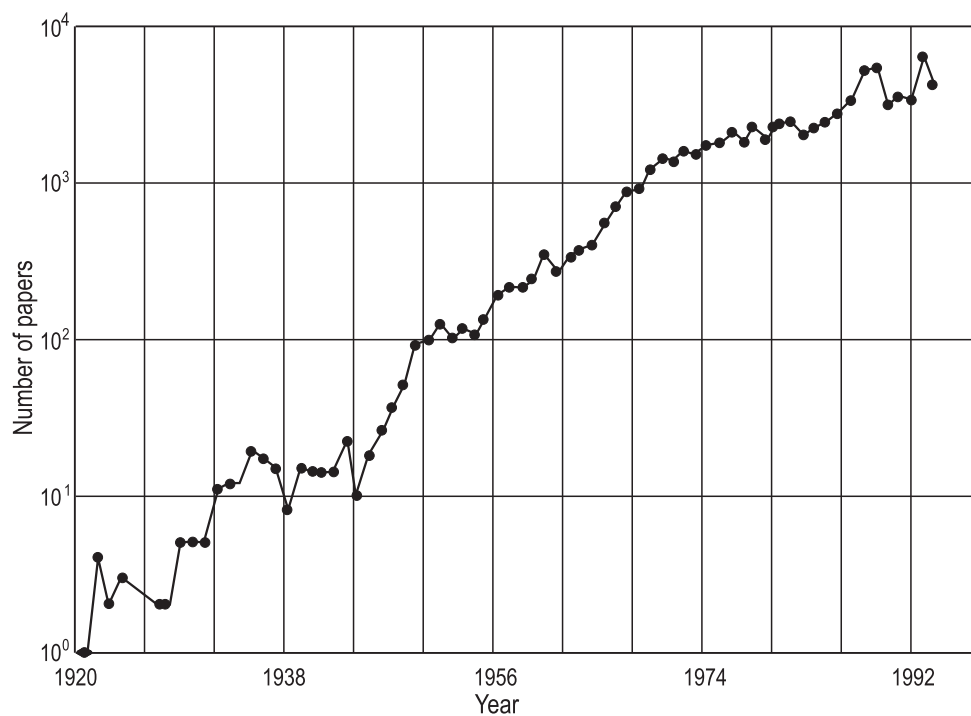


Fig. ID-3. Number of research papers on ferroelectrics and related substances published within each year. Prepared by K. Deguchi on the basis of [93Toy] (cf. IA).

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 (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.

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 ΔH are arranged according to the letters following Δ (e.g. ΔH is to be found in the place of H , not Δ).

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	LT	low temperature
I, II, III, ...	names of phases	mon	monoclinic
A, AF	antiferroelectric	NMR	nuclear magnetic resonance
(A)	possibility of being antiferroelectric	NQR	nuclear quadrupole resonance
A, B, C, ...	symbol for atom, various compositions	orth	orthorhombic
ac	alternating current	P	paraelectric
cub, c	cubic	(P)	possibility of being paraelectric
DTA	differential thermal analysis	pc	pseudocubic
dc	direct current	pol	polarization
ESR	electron spin resonance	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
LO	longitudinal optic	TO	transverse optic

c) Symbols and units

Symbols	Units	Definitions
A	numeral	Absorption
A	kg kg^{-1} , kg m^{-3} , wt%	solubility
A, B	m^{-1}	HFS parameters
${}^nA_{ij}$	A m^{-1}	hyperfine splitting tensor, n : nuclear mass number
nA_i	A m^{-1}	principal value of hyperfine splitting tensor, n : nuclear mass number
${}^nA_{ }, {}^nA_{\perp}$	A m^{-1}	hyperfine splitting parameters in axial symmetry, n : nuclear mass number
ΔA	K^{-1}	change in slope of $1/\kappa$ vs. T curve.
a	m^{-1}	FS parameter
$\mathbf{a}, \mathbf{b}, \mathbf{c}$	\AA	unit cell vector
a, b, c	\AA	length of unit cell edges
$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$	\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	\AA^2	isotropic temperature parameter [cf. Eq. (e) in Introduction]
B_{ij}	numeral	anisotropic temperature parameter [cf. Eq. (a) in Introduction]
b	m^{-1}	FS parameter
b_{ij}	numeral	anisotropic temperature parameter [cf. Eq. (b) in Introduction]
c	m s^{-1}	light velocity in vacuum ($c = 2.99792458 \cdot 10^8 \text{ m s}^{-1}$)
C	K	Curie-Weiss constant with regard to κ : $\kappa = \kappa_{\infty} + C/(T - \Theta_p)$
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	N m^{-2}	longitudinal elastic modulus
c_s	N m^{-2}	shear elastic modulus
$c_{\lambda\mu}$	N m^{-2}	elastic stiffness
D	m^{-1}	FS parameter
D	numeral	dissipation factor
\mathbf{D}	C m^{-2}	electric displacement
d	m	thickness of specimen
d	\AA	bond length
d_{hkl}	\AA	interplanar spacing of planes (hkl)
$d_{i\lambda}$	C N^{-1}	piezoelectric strain constant
$d_{i\lambda}$	m V^{-1}	susceptibility for second harmonic generation (see section IC)
E	eV	energy
E	N m^{-2}	Young's modulus
E	m^{-1}	FS parameter
\mathbf{E}	V m^{-1}	electric field strength
$\Delta E, \Delta E_{\text{quad}}$	m s^{-1}	quadrupole splitting in Mössbauer spectrum
E_{bias}	V m^{-1}	bias field
E_c	V m^{-1}	coercive field
E_{crit}	V m^{-1}	critical field
E_G	eV	energy separation, band gap
e	C	charge of electron ($ e = 1.60217733(49) \cdot 10^{-19} \text{ C}$)
\mathbf{e}	m^{-1}	polarization vector of phonon
$e_{i\lambda}$	C m^{-2}	piezoelectric stress constant
$e^2 q Q / h$	Hz	nuclear quadrupole coupling constant
$e Q \phi_{ij} / h$	Hz	component of nuclear quadrupole coupling tensor

Symbols	Units	Definitions
F	m^{-1}	FS parameter
$F.M._{R_I}$	C m J^{-1}	$F.M._{R_I} = p_i \rho^{-1} c_p^{-1}$, figure of merit for current responsivity
$F.M._{R_V}$	C m J^{-1}	$F.M._{R_V} = p_i \rho^{-1} c_p^{-1} \kappa^{-1}$, figure of merit for voltage responsivity
$F.M._N$	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
Δf_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	A m^{-1}	magnetic field strength
\mathbf{H}	J m^{-3}	spin Hamiltonian
H_c	A m^{-1}	coercive field strength, coercive force
H_V	kg m^{-2}	Vickers hardness number
ΔH	A m^{-1}	magnetic resonance half width
$\Delta'H$	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
ΔH_{pp}	A m^{-1}	line width in ESR
ΔH_i	A m^{-1}	line shift in ESR
$\delta'H$	A m^{-1}	magnetic resonance line separation
h	J s	Planck constant ($h = 6.6260755(40) \cdot 10^{-34} \text{ J s}$)
$h_{i\lambda}$	N C^{-1}	piezoelectric stress constant
I	A	electric current
I	J s^{-1}	scattering intensity
I	numeral	nuclear spin quantum number
I_{hkl}	J s^{-1}	integrated intensity of Bragg reflection (hkl)
I_s	A	switching current
J	A	photovoltaic current
\mathbf{J}	V s m^{-2}	magnetic polarization, $\mathbf{J} = \mathbf{B} - \mu_0 \mathbf{H}$
j	A m^{-2}	electric current density
k	J K^{-1}	Boltzmann constant ($k = 1.380658(12) \cdot 10^{-23} \text{ J K}^{-1}$)
k	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
$\Delta l/l$	m m^{-1}	elongation per unit length
l_{ij}	m	coherence length
M	numeral	molecular weight
\mathbf{M}	A m^{-1}	magnetization, $\mathbf{M} = \mathbf{B}/\mu_0 - \mathbf{H}$

Symbols	Units	Definitions
M_s	A m^{-1}	spontaneous magnetization
$M_{\lambda\mu}$	$\text{m}^4 \text{C}^{-2}$	quadratic electrooptic constant for \mathbf{P}
m_0	kg	electron mass ($m_0 = 9.1093897(54) \cdot 10^{-31} \text{ kg}$)
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 ($n_\alpha < n_\beta < n_\gamma$)
Δn	numeral	birefringence
P	W m^{-2}	light intensity
P	C m^{-2}	dielectric polarization
P_L	C m^{-2}	longitudinal polarization
P_{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_{eff}	μ_B	effective magnetic moment of atom or ion
p_i	$\text{C K}^{-1} \text{m}^{-2}$	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
ΔQ_m	J mol^{-1}	transition heat per mole
$Q_{\lambda\mu}$	$\text{m}^4 \text{C}^{-2}$	electrostrictive constant for \mathbf{P}
q	m^{-1}	wave number ($2\pi/\lambda$)
\mathbf{q}	m^{-1}	wave number vector
R	Ω	resistance
R	numeral	reflectivity
R	numeral, %	discrepancy index (or reliability factor)
R_H	$\text{m}^3 \text{C}^{-1}$	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	$\text{J K}^{-1} \text{m}^{-3}$	entropy per unit volume
S_m	$\text{J K}^{-1} \text{mol}^{-1}$	entropy per mole
ΔS_m	$\text{J K}^{-1} \text{mol}^{-1}$	transition entropy per mole
\mathbf{S}	m m^{-1}	strain tensor
S_{ij}	m m^{-1}	component of strain tensor
S_λ	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
$s_{\lambda\mu}$	$\text{m}^2 \text{N}^{-1}$	elastic compliance
T	K, °C	temperature

Symbols	Units	Definitions
T	numeral	transmission
T_g	K, °C	glas transition temperature
T_{melt}	K, °C	melting point
T_x	K, °C	crystallization onset temperature
\mathbf{T}	N m^{-2}	stress tensor
T_{ij}	N m^{-2}	component of stress tensor
T_λ	N m^{-2}	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
ΔT_{irrev}	K, °C	irreversible electrocaloric temperature change
ΔT_{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
ΔU	eV, J mol^{-1}	activation energy
U_{ij}	\AA^2	anisotropic temperature parameter [cf. Eq. (d) in Introduction]
V	V	voltage
V	° ' ,	1/2 (optical axial angle)
V	\AA^3	volume of unit cell
V	° $\text{m}^{-1} \text{T}^{-1}$	Verdet constant
V_m	\AA^3	volume for formula unit
V_π	V	half-wave voltage
V_{zz}	V m^{-2}	electric field gradient
ν	m s^{-1}	sound velocity
ν	m s^{-1}	velocity of absorber in Mössbauer effect
ν_0	m s^{-1}	effective amplitude of vibration velocity
ν_m	$\text{m}^3 \text{mol}^{-1}$	molar volume
X, Y, Z	$\text{\AA}, \text{m}$	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	$\text{\AA}, \text{m}$	principal axes of tensor ellipsoid
y	numeral	normalized yield
Z	numeral	number of formula units per cell
Z_{vac}	numeral	number of vacancies
α	$\text{m}^{-1}, \text{dB m}^{-1}, \text{neper m}^{-1}$	acoustic absorption coefficient
α	dB s^{-1}	ultrasonic attenuation
α	m^{-1}	optical absorption coefficient
α	$\text{m}^2 \text{s}^{-1}$	thermal diffusivity
α	° ' ,	rhombohedral angle
α_{ij}	K^{-1}	linear thermal expansion coefficient
α_κ	numeral	temperature coefficient of κ
α, β, γ	° ' ,	interaxial angles: $b \wedge c, c \wedge a, a \wedge b$
$\alpha^*, \beta^*, \gamma^*$	° ' ,	interaxial angles: $b^* \wedge c^*, c^* \wedge a^*, a^* \wedge b^*$
β_{ij}	\AA^2	anisotropic temperature parameter [cf. Eq. (c) in Introduction]

Symbols	Units	Definitions
Γ	Hz	full width at half maximum of spectral line
Γ	Hz	damping parameter
Γ	m s^{-1}	line width of Mössbauer absorption line (half width at half maximum)
γ	$\text{m A}^{-1} \text{ s}^{-1}$	gyromagnetic ratio
γ	K^{-1}	cubic thermal expansion coefficient
δ	m s^{-1}	isomer shift
δ	rad	dielectric loss angle
$\tan \delta$	numeral	dielectric loss tangent: $\tan \delta = \kappa''/\kappa'$
ε	F m^{-1}	permittivity, $D = \varepsilon E$
ε_{ij}	F m^{-1}	components of dielectric permittivity tensor
ε_0	F m^{-1}	permittivity of vacuum ($\varepsilon_0 = 8.854187817 \cdot 10^{-12} \text{ F m}^{-1}$)
ζ	$\text{V m}^9 \text{ C}^{-5}$	coefficient of power series expansion of electric field strength: $E = (1/\chi_p)P + \xi P^3 + \zeta P^5$
ζ	numeral	reduced wave vector coordinate
η	numeral	asymmetry parameter
Θ	K, °C	transition temperature
$\Theta_{\text{II-I}}$	K, °C	transition temperature between the phases II and I
Θ_c	K, °C	superconducting transition temperature
Θ_f	K, °C	ferroelectric transition temperature
Θ_a	K, °C	antiferroelectric transition temperature
Θ_p	K, °C	paraelectric Curie temperature in the Curie-Weiss law
$\Theta_{\text{f magn}}$	K, °C	ferromagnetic transition temperature
Θ_N	K, °C	antiferromagnetic Néel temperature
$\Theta_{\text{p magn}}$	K, °C	paramagnetic Curie temperature in the Curie-Weiss law
Θ_ϕ	K, °C	phase match temperature
$\Delta\Theta$	K, °C	shift of phase transition temperature
θ	°	tilt angle
θ_B	rad, °	Bragg angle (scattering angle = $2\theta_B$)
κ	numeral	dielectric constant: $\kappa = \varepsilon/\varepsilon_0$
κ_0	numeral	static dielectric constant
κ_∞	numeral	temperature-independent term in Curie-Weiss law: $\kappa = \kappa_\infty + C/(T - \Theta_p)$
κ', κ''	numeral	real and imaginary parts of complex dielectric constant: $\kappa = \kappa' + i\kappa''$
κ_{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
λ	m	wave length
λ	$\text{J s}^{-1} \text{ m}^{-1} \text{ K}^{-1}$	thermal conductivity
$1/\lambda$	m^{-1}	wave number per unit length
λ, μ, ν	numeral	direction cosines
μ_0	H m^{-1}	permeability of vacuum ($\mu_0 = 4\pi \cdot 10^{-7} \text{ H m}^{-1}$)
μ_B	J T^{-1}	Bohr magneton ($\mu_B = 9.2740154(31) \cdot 10^{-24} \text{ J T}^{-1}$)
μ_n	J T^{-1}	nuclear magneton ($\mu_n = 5.0507866(17) \cdot 10^{-27} \text{ J T}^{-1}$)
μ_H	$\text{m}^2 \text{ V}^{-1} \text{ s}^{-1}$	Hall mobility
ν	Hz	frequency (mainly used in optical properties)
$\Delta\nu$	Hz	splitting of the resonance frequencies
$\Delta\nu$	Hz	frequency shift

Symbols	Units	Definitions
ν_H	Hz	frequency of resonance field
ν_L	Hz	Larmor frequency
ν_c	Hz	correlation frequency
$\delta\nu$	Hz	half width at half maximum
$\delta\nu$	Hz	doublet separation of NQR spectrum
ξ	$V\ m^5\ C^{-3}$	coefficient of power series expansion of electric field strength: $E = (1/\chi_p)P + \xi P^3 + \zeta P^5$
ξ, η, ζ	numeral	fractional coordinates in the reciprocal unit cell
$\Pi_{\lambda\mu}$	$m^2\ N^{-1}$	piezooptic constant for T
$\pi_{i\lambda}$	$m^2\ N^{-1}$	piezoresistive constant
ρ	$\Omega\ m$	resistivity
ρ	$^\circ\ m^{-1}$	specific rotatory power
ρ	$kg\ m^{-3}$	density
ρ_a	$kg\ m^{-3}$	apparent density
ρ_e	\AA^{-3}	electron density (number of electrons per \AA^3)
σ_{ph}	$\Omega^{-1}\ m^{-1}$	photoconductivity
ρ_r	$kg\ m^{-3}$	relative density
ρ_X	$kg\ m^{-3}$	X-ray density
ρ_{li}	$m^2\ C^{-1}$	electrooptic constant for P
σ	$\Omega^{-1}\ m^{-1}$	conductivity
σ	Ω^{-1}	surface conductivity
σ	$C\ m^{-1}$	charge density
σ	numeral	standard deviation in fractional coordinates of atomic position
σ	\AA^2	standard deviation in temperature parameter
σ	$A\ m^2\ kg^{-1}$	magnetic moment per unit mass, specific magnetization
σ_m	$A\ m^2\ mol^{-1}$	magnetic moment per mole
τ	sec, s	dielectric relaxation time
τ_c	sec, s	correlation time
ϕ	$^\circ, '$	rotation angle
ϕ_o	$^\circ, '$	rotation angle of optical indicatrix
ϕ_{ij}	$V\ m^{-2}$	components of the electric field gradient tensor
χ	$F\ m^{-1}$	electric susceptibility
χ_p	$F\ m^{-1}$	paraelectric susceptibility
$\chi_{magn\ m}$	$m^3\ mol^{-1}$	molar magnetic susceptibility
$\chi_{magn\ \rho}$	$m^3\ kg^{-1}$	mass magnetic susceptibility, specific susceptibility
χ_{me}	$s\ m^{-1}$	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	S	at strain S
D	at electric displacement D	<i>T</i>	at temperature <i>T</i>
E	at field strength E	T	at stress T
P	at polarization P		

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
ρ	per gram (only for magnetic quantities)	ext	external
HT	high temperature	fmagn	ferromagnetic
i, j, k	numerals (1...3)	hex, h	hexagonal
λ, μ, ν	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	magnetolectric
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	10^2 cm	10^2 cm
Mass	<i>m</i>	kg	10^3 g	10^3 g
Time	<i>t</i>	s	1 s	1 s
Density	ρ	kg m^{-3}	10^{-3} g cm^{-3}	10^{-3} g cm^{-3}
Electric field strength	<i>E</i>	V m^{-1}	10^{-4} / 3esu	10^6 emu
Electric displacement	<i>D</i>	C m^{-2}	$12\pi \cdot 10^5$ esu	$4\pi \cdot 10^{-5}$ emu
Dielectric polarization	<i>P</i>	C m^{-2}	$3 \cdot 10^5$ esu	10^{-5} emu
Dielectric constant	κ	dimensionless	1 (dimensionless)	1 (dimensionless)
Piezooptic constant	$p_{\lambda\mu}$	dimensionless	1 (dimensionless)	1 (dimensionless)

(continued)

Table IE-3. (continued)

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

IF Survey of contained data

Each chapter of this volume corresponds to one family consisting of similar substances. This Subvolume A contains nineteen oxide families and thus nineteen chapters, as listed in table of contents. 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: The 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 this Subvolume 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 (κ vs. <i>T</i> , Curie-Weiss law constants, κ vs. <i>p</i> , κ vs. two- or one-dimensional pressure, κ vs. frequency, phase diagram in regard to <i>p</i> and E_{bias}).
b	Nonlinear dielectric properties (effect of E_{bias} on κ , values of ξ and ζ).
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)

Table IF-1. (continued)

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	Piezooptic 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).

IG Outline of Subvolume B: Non-oxides

Table IG-1. Substance families contained in Subvolume B: Non-oxides

Part 1: Inorganic crystals other than oxides

20	SbSI family [T. Yagi]
21	TlS [Y. Shiozaki]
22	TlInS ₂ family [Y. Shiozaki]
23	Ag ₃ AsS ₃ family [K. Deguchi]
24	Sn ₂ P ₂ S ₆ family [K. Deguchi]
25	KNiCl ₃ family [Y. Shiozaki]
26	BaMnF ₄ family [K. Deguchi]
27	HCl family [K. Gesi]
28	NaNO ₂ family [K. Gesi]
29	CsCd(NO ₂) ₃ family [K. Hasebe, T. Asahi]
30	KNO ₃ family [K. Gesi]
31	LiH ₃ (SeO ₃) ₂ family [M. Komukae, T. Osaka]
32	KIO ₃ family [K. Hasebe, T. Asahi]
33	KH ₂ PO ₄ (KDP) family [E. Nakamura, M. Komukae, T. Osaka]
34	PbHPO ₄ family [K. Gesi]
35	KTiOPO ₄ family [T. Hikita]
36	CsCoPO ₄ family [N. Nakatani]
37	NaTh ₂ (PO ₄) ₃ family [Y. Shiozaki]
38	Te(OH) ₆ · 2NH ₄ H ₂ PO ₄ · (NH ₄) ₂ HPO ₄ [E. Nakamura]
39	(NH ₄) ₂ SO ₄ family [K. Deguchi, K. Hasebe, K. Gesi, T. Asahi]
40	NH ₄ HSO ₄ family [T. Yagi]
41	NH ₄ LiSO ₄ family [T. Yagi]
42	(NH ₄) ₃ H(SO ₄) ₂ family [K. Gesi]
43	Langbeinite-type family [T. Hikita]
44	Lecontite (NaNH ₄ SO ₄ · 2H ₂ O) family [M. Komukae, T. Osaka]
45	Alum (NH ₄ Fe(SO ₄) ₂ · 12H ₂ O) family [M. Komukae, T. Osaka]
46	GASH (C(NH ₂) ₃ Al(SO ₄) ₂ · 6H ₂ O) family [K. Gesi]
47	Colemanite (Ca ₂ B ₆ O ₁₁ · 5H ₂ O) [M. Komukae, T. Osaka]
48	K ₄ Fe(CN) ₆ · 3H ₂ O family [M. Komukae, T. Osaka]
49	K ₃ BiCl ₆ · 2KCl · KH ₃ F ₄ [Y. Shiozaki]
M15	SnTe group [Y. Akishige]
M16	PbN ₆ [E. Nakamura]
M17	Sb ₂ S ₃ [T. Yagi]
M18	Sb ₅ O ₇ I [T. Yagi]
M19	H ₂ O [K. Nakatani]
M20	KOH group [E. Nakamura]
M21	KSCN [E. Nakamura]
M22	Na ₃ Sc ₂ (PO ₄) ₃ [E. Nakamura]
M23	H ₂ (UO ₂) ₂ (AsO ₄) ₂ · 8H ₂ O [E. Nakamura]
M24	Li(N ₂ H ₅)SO ₄ group [E. Nakamura]
M25	N(CH ₃) ₄ HSO ₄ · H ₂ O [E. Nakamura]
M26	Ag ₂ H ₃ IO ₆ group [E. Nakamura]
M27	MNbWO ₆ · nH ₂ O group (M = Rb, Tl) [E. Nakamura]
M28	NH ₄ PF ₆ · NH ₄ F [E. Nakamura]

Part 2: Organic crystals, liquid crystalline and high polymer ferroelectrics

50	SC(NH ₂) ₂ family [Y. Shiozaki, T. Ashi]
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- 51 $\text{CCl}_3\text{CONH}_2$ [Y. Shiozaki]
 52 $\text{Cu}(\text{HCOO})_2 \cdot 4\text{H}_2\text{O}$ [M. Komukae, T. Osaka]
 53 $\text{N}(\text{CH}_3)_4\text{HgCl}_3$ family [M. Adachi]
 54 $\text{CH}_3\text{NH}_3\text{AlCl}_4$ family [Y. Shiozaki]
 55 $[(\text{CH}_3)_2\text{NH}_2]_2\text{CoCl}_4$ family [K. Hasebe, T. Asahi]
 56 $[(\text{CH}_3)_2\text{NH}_2]_3\text{Sb}_2\text{Cl}_9$ family [K. Hasebe, T. Asahi]
 57 $(\text{CH}_3\text{NH}_3)_5\text{Bi}_2\text{Cl}_{11}$ family [K. Hasebe, T. Asahi]
 58 $\text{DSP} (\text{Ca}_2\text{Sr}(\text{CH}_3\text{CH}_2\text{COO})_6)$ family [E. Nakamura]
 59 $\text{CH}_2\text{ClCOONH}_4$ family [E. Nakamura]
 60 $\text{TGS} ((\text{NH}_2\text{CH}_2\text{COOH})_3 \cdot \text{H}_2\text{SO}_4)$ 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 Liquid crystals [H. Takezoe, Y. Ishibashi, R. Nozaki, E. Nakamura]
 72 High polymers [T. Furakawa, 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]

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