

ANSI IEEE
C83.3-1951 Std 176-1949
(Reaffirmed 1972) (Reaffirmed 1971)

STANDARDS ON PIEZOELECTRIC CRYSTALS, 1949

Reprinted from the PROCEEDINGS OF THE I.R.E.
VOL. 37, NO. 12, DECEMBER, 1949

PRINTED IN THE U.S.A.

Standards on PIEZOELECTRIC CRYSTALS, 1949*

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INTRODUCTION

In 1945 a report entitled "Standards on Piezoelectric Crystals: Recommended Terminology" was prepared by the Committee on Piezoelectric Crystals and issued by the Institute. The present report involves not only much new material, but also a revision of certain portions of the earlier report.

Part I of the 1945 report (corresponding to Part 1 of this Standard) remains unchanged, with the following exceptions: The use of left-handed axes for left crystals is now abandoned (see Sections 1.9, and 1.11 to 1.14); and the 1945 rules for rotated plates are now supplanted by the rules in the present report.

In Part II (corresponding to Part 2 of this Standard), Sections 11 and 13 have been revised. Otherwise, Part II

remains in effect. The introduction of new crystals, some belonging to classes for which no satisfactory conventions have existed, makes desirable a self-consistent set of conventions, sufficiently comprehensive to include all piezoelectric crystal classes. This necessitates certain changes in the definitions of the axes of quartz and in the algebraic signs of piezoelectric and elastic constants, as described in Sections 1.12 to 1.14. These changes result not only in agreement with the crystallographers, but, fortunately, in better conformity with shop practice as it has developed.

Part 3 of the new Standard presents basic equations, symbols, and units of piezoelectric theory. It has been prepared in view of the growing tendency to express

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elastic stress and strain as dependent upon the electric displacement, rather than upon the electric field, and also in view of the increasing use of mks units. The formulation in terms of displacement is especially useful in cases where there is a gap between crystal and electrodes, also in dealing with crystals whose constants show a marked dependence on temperature. In the latter case it is found that the "constants" have more nearly constant values when expressed in terms of displacement than in terms of field.

When there is no gap between crystal and electrodes it is often found more convenient to use Voigt's formulation, with the piezoelectric constants expressed in terms of electric field strength rather than displacement.

The equations are interconvertible. The Voigt piezoelectric constants d and e are related to the more recent constants g and h by the dielectric constant. For some purposes it is convenient to use expressions involving combinations of constants from both formulations. In doing so it is necessary, of course, to use the same system of units, esu or mks.

AUTHORSHIP AND ACKNOWLEDGMENT

This Standard is the result of several years of conferences involving all of the members of the Committee. Its form and its completeness, which in effect make it

an introduction to the formal treatment of piezoelectricity, come from the fact that it is basically a collection of several papers prepared for the Committee by individual members and their collaborators serving as subcommittees. There would have been entire justification for the separate publication of these papers by their individual authors, but it has been the view of the Committee that the advantages of unification into a system such as the Standard is intended to establish could best be gained by bringing all papers into a common publication with agreement as to symbols, conventions, and equations.

The authorship of the several parts of the Standard is as follows: Part 1 is an elaboration of memoranda prepared for the Committee by W. L. Bond, entitled "Crystal Axis Nomenclature," October 25, 1946, and "Axes For Triclinic Crystals," June 16, 1947. Part 2 stems from a memorandum by W. L. Bond of August 19, 1946, on "Crystal Rotation Systems." Part 3 is an expansion of a memorandum by Paul L. Smith, "The Piezoelectric Relations, Symbols and Units," June 3, 1946, in which he had the collaboration of H. G. Baerwald of the Brush Development Company. The adopted formulation of the theory is based on equations first presented by the latter in a wartime report¹ to the NDRC.

¹ H. G. Baerwald, OSRD Report No. 287, Contract No. OEMsr-120, 1941.

1. Definitions of Axes for Piezoelectric Crystals

1.1 Crystals and Their Classification

For the guidance of those who are not familiar with crystallography, the following summary of those principles to which reference will be made later in this Standard may be helpful.

The term "crystal" is usually applied to solids that possess structural symmetry. In a crystal the atoms may be thought of as occurring in small groups, all groups exactly alike, similarly oriented, and regularly aligned in all three dimensions. If each group is regarded as bounded by a parallelepiped, the latter can be looked upon as one of the ultimate building blocks of the crystal; they are stacked together in all three dimensions without any spaces between. Such a building block is called a *unit cell*. Since the choice of the particular set of atoms to form a unit cell is arbitrary, it is evident that there is a wide range of choice in the shape and

dimensions of the unit cell. In practice, that unit cell is selected which is most simply related to the actual crystal faces and X-ray reflections, and which has the symmetry of the crystal itself. Except in a few special cases the unit cell has the smallest possible size.

Depending on their degrees of symmetry, crystals are commonly classified in seven *systems*: triclinic (the least symmetrical), monoclinic, orthorhombic, tetragonal, hexagonal, trigonal, and isometric. Some authorities, however, treat trigonal crystals as a division of the hexagonal system.

The seven systems in turn are divided into point-groups (classes) according to their symmetry with respect to a point. There are thirty-two such classes, of which twelve are of too high a degree of symmetry to show piezoelectric properties. Thus twenty classes can be piezoelectric. Every system contains at least one piezoelectric class.

1.2. General

In determining a suitable nomenclature for the many new crystals that are finding their way into the piezoelectric field, it seems wise to make use of the nomenclature of the highly developed science of crystallography. This facilitates the use of data already recorded by crystallographers. Such data are, for example, atomic cell dimensions and angles, optical properties, and interfacial angles, all of which can be useful for establishing orientations of piezoelectric plates. In crystallography, the properties of a crystal are described in terms of the natural co-ordinate system provided by the crystal itself. The axes of this natural system are the edges of the unit cell. In a cubic crystal these axes are of equal length and are mutually perpendicular; in a triclinic crystal they are of unequal lengths and no two are mutually perpendicular.

The faces of any crystal are all parallel to planes whose intercepts on the natural axes a , b , c are small multiples of unit distances or else infinity, so that their reciprocals, when multiplied by a small common factor, are all small integers or zero. These are the indices of the planes. In this nomenclature we have, for example, faces (100), (010), (001), also called the a , b , c faces, respectively; in the orthorhombic, tetragonal, and isometric systems these faces are normal to the a , b , c axes. Other examples are faces (111) (the unit face), (121), etc. As referred to a set of rectangular axes X , Y , Z , these indices will in general be irrational except for cubic crystals.

On the other hand, the theoretical treatment of electricity and elasticity, which is fundamental in piezoelectric applications, has been developed with rectangular axes. One must therefore adopt some arbitrary relation between the a , b , c axes of crystallography and the rectangular X , Y , Z axes. Unless all workers in the field agree to use the same nomenclature, there will be great confusion. Data expressed in terms of one abc - XYZ relation look very different from the same data in terms of another abc - XYZ relation.

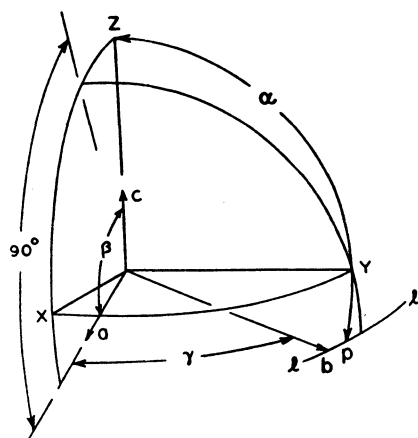


Fig. 1—Axes of triclinic crystals.
The line $l-l$ is on a small circle with pole Z and angle α . For b to left of p , $\gamma < 90^\circ$. For b to right of p , $\gamma > 90^\circ$.

1.3. The Triclinic System

If there are neither symmetry axes nor symmetry planes present in a crystal, it is triclinic. The lengths of the three axes are in general unequal, and the angles α , β , and γ are also unequal. α , β , γ are the angles between b and c , c and a , and a and b , respectively, as shown in Fig. 1. Fig. 2, a triclinic crystal, shows that

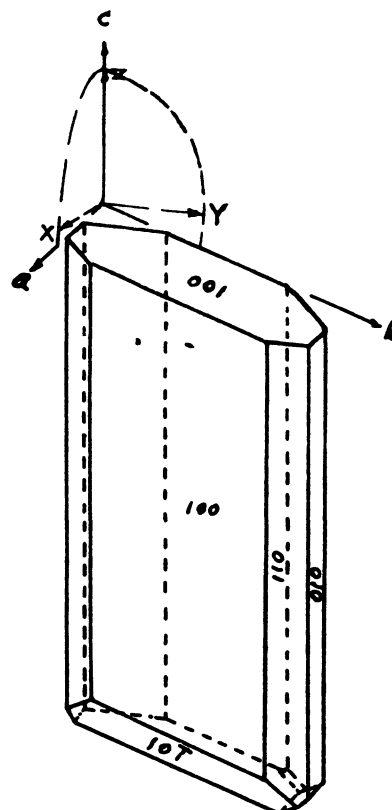


Fig. 2—Aminoethyl ethanolamine hydrogen d -tartrate, triclinic, class 1.
The Z axis is along c , Y normal to (010), X perpendicular to Y and Z .

the a axis has the direction of the intersection of the faces b and c (extend the faces to intersection if necessary), the b axis has the direction of the intersection of faces c and a , the c axis has the direction of the intersection of faces a and b . According to the best current usage the positive directions of a , b , and c are taken so as to make α greater than 90° , and β also greater than 90° . This convention determines uniquely the positive senses of all axes. (Many old works record the complementary angle, i.e., the angle between $-a$ and $+c$ as β .) The a , b , and c axes are in general to be chosen as the three shortest noncoplanar interatomic distances, with c the shortest unit distance, b the longest.

1.3.1. The X , Y , Z axes

The most logical relation is that which associates the X , Y , Z axes most closely with the a , b , c axes, respec-

tively. There are six equally simple ways of completing the specification: X along a and Y in the ab plane; X along a and Z in the ac plane; Y along b and X in the ab plane; Y along b and Z in the bc plane; Z along c and Y in the bc plane; or Z along c and X in the ac plane. In physics and technology Z is commonly pictured as the vertical axis, while in crystallography c is usually so pictured. Hence we take Z along c and have only the choice of Y in the bc plane or X in the ac plane. The choice now accepted is to let Y be normal to the ac plane; this automatically places X in the ac plane.

The rules for the rectangular axes, together with their positive directions, are summarized as follows (see Figs. 1 and 2):

- + Z is parallel to + c , hence parallel to the (100) and (010) planes.
- + X is perpendicular to c in the ac plane, pointing in the general direction of + a . X is thus parallel to (010).
- + Y is normal to the ac plane (010), pointing in the general direction of + b , and forming a right-handed axial system with Z and X .

1.4. The Monoclinic System

If a crystal has but a single axis of twofold symmetry, or but a single plane of reflection symmetry, or both, it belongs to the monoclinic system. Either the twofold axis or the normal to the plane of symmetry (they are the same if both exist, and this direction is called the unique axis in any case) is taken as the b axis. Of the two remaining axes, modern crystallographers always make c the smaller. The angle β between + a and + c is always obtuse (a special convention has to be adopted when this angle is obtuse at some temperatures, acute at others). This convention determines uniquely the positive directions of all axes for classes 2 and 2/ m . In class m there are two alternatives. The choice between them is indicated in Section 1.16. Since the axes chosen by early workers may not give the smallest possible cell, a new cell with a smaller volume can be chosen.

Many physicists seem to prefer to make Z the unique axis of monoclinic crystals. This is the convention adopted by Voigt, and continued by Cady in his book "Piezoelectricity."² Nevertheless, in most crystallographic literature b is taken as the unique axis in the monoclinic system. Henceforth " Z along c , Y along b " is to be the standard abc - XYZ relation for monoclinic crystals, as illustrated in Fig. 3. According to this convention, with the unique axis b taken as the Y axis, the stresses T and strains S are related through the matrix

equations $S = sT$ and $T = cS$, where the compliance constant s takes the form³

$$s = \begin{vmatrix} s_{11} & s_{12} & s_{13} & 0 & s_{15} & 0 \\ s_{12} & s_{22} & s_{23} & 0 & s_{25} & 0 \\ s_{13} & s_{23} & s_{33} & 0 & s_{35} & 0 \\ 0 & 0 & 0 & s_{44} & 0 & s_{46} \\ s_{15} & s_{25} & s_{35} & 0 & s_{55} & 0 \\ 0 & 0 & 0 & s_{46} & 0 & s_{66} \end{vmatrix} \quad (1)$$

The stiffness constant c takes an analogous form. Also, electric displacement and elastic stress are related through the matrix equation $D = dT$, where the piezoelectric strain-constant d takes the form, for class 2 (Y a twofold axis),

$$d = \begin{vmatrix} 0 & 0 & 0 & d_{14} & 0 & d_{16} \\ d_{21} & d_{22} & d_{23} & 0 & d_{25} & 0 \\ 0 & 0 & 0 & d_{34} & 0 & d_{36} \end{vmatrix} \quad (2)$$

while for class m (a plane of reflection-symmetry perpendicular to Y)

$$d = \begin{vmatrix} d_{11} & d_{12} & d_{13} & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{24} & 0 & d_{26} \\ d_{31} & d_{32} & d_{33} & 0 & d_{35} & 0 \end{vmatrix} \quad (3)$$

The matrices (1), (2), and (3) replace those that have hitherto been in common use according to Voigt's convention. To each elastic or piezoelectric constant on the new convention there corresponds one on the old, with the same numerical value.

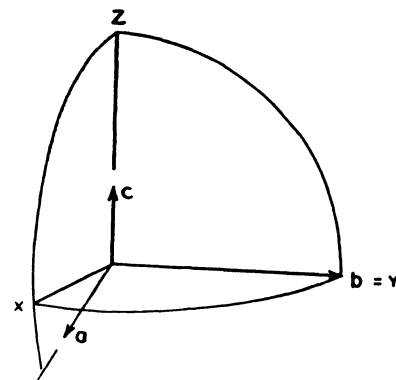


Fig. 3—Axes of monoclinic crystals.
 a and c are perpendicular to b but not to each other.

For comparison with the new matrices (1), (2), and (3), the corresponding expressions according to Voigt's

² W. G. Cady, "Piezoelectricity." McGraw-Hill Book Co., New York, N. Y., 1946

³ See part 3 of this Standard.

convention will now be given. The Voigt matrix for *Monoclinic, class m* elastic compliance, now abandoned, is

$$s = \begin{bmatrix} s_{11} & s_{12} & s_{13} & 0 & 0 & s_{16} \\ s_{12} & s_{22} & s_{23} & 0 & 0 & s_{26} \\ s_{13} & s_{23} & s_{33} & 0 & 0 & s_{36} \\ 0 & 0 & 0 & s_{44} & s_{45} & 0 \\ 0 & 0 & 0 & s_{45} & s_{55} & 0 \\ s_{16} & s_{26} & s_{36} & 0 & 0 & s_{66} \end{bmatrix} \quad (4)$$

with an analogous form for c .

For class 2, the Voigt matrix (in which Z is a twofold axis), now abandoned, is

$$d = \begin{bmatrix} 0 & 0 & 0 & d_{14} & d_{15} & 0 \\ 0 & 0 & 0 & d_{24} & d_{25} & 0 \\ d_{31} & d_{32} & d_{33} & 0 & 0 & d_{36} \end{bmatrix}, \quad (5)$$

while for class m (reflection-plane perpendicular to Z) the Voigt matrix, now abandoned, is

$$d = \begin{bmatrix} d_{11} & d_{12} & d_{13} & 0 & 0 & d_{16} \\ d_{21} & d_{22} & d_{23} & 0 & 0 & d_{26} \\ 0 & 0 & 0 & d_{34} & d_{35} & 0 \end{bmatrix} \quad (6)$$

If we know the s and d matrices for Voigt's convention, we can put them in standard form by means of the following matrices:

$$s = \begin{bmatrix} s_{22}' & s_{23}' & s_{12}' & 0 & s_{26}' & 0 \\ s_{23}' & s_{33}' & s_{13}' & 0 & s_{36}' & 0 \\ s_{12}' & s_{13}' & s_{11}' & 0 & s_{16}' & 0 \\ 0 & 0 & 0 & s_{55}' & 0 & s_{45}' \\ s_{26}' & s_{36}' & s_{16}' & 0 & s_{66}' & 0 \\ 0 & 0 & 0 & s_{45}' & 0 & s_{44}' \end{bmatrix} \quad (7)$$

where the subscripts of the primed values are those according to Voigt.

Monoclinic, class 2

$$d = \begin{bmatrix} 0 & 0 & 0 & d_{26}' & 0 & d_{24}' \\ d_{32}' & d_{33}' & d_{31}' & 0 & d_{36}' & 0 \\ 0 & 0 & 0 & d_{24}' & 0 & d_{14}' \end{bmatrix} \quad (8)$$

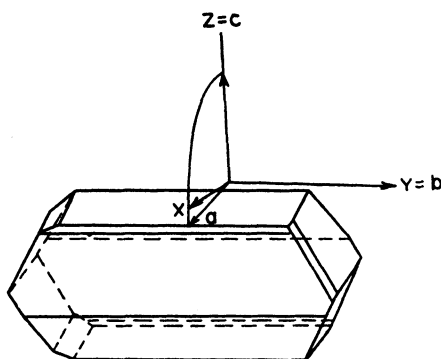


Fig. 4—Lithium sulfate monohydrate, a monoclinic crystal, class 2. The specimen here shown is left-handed. On extension along the b axis, the $+b$ end becomes negatively charged.

$$d = \begin{bmatrix} d_{22}' & d_{23}' & d_{31}' & 0 & d_{26}' & 0 \\ 0 & 0 & 0 & d_{33}' & 0 & d_{34}' \\ d_{12}' & d_{13}' & d_{11}' & 0 & d_{16}' & 0 \end{bmatrix} \quad (9)$$

Examples of monoclinic crystals are shown in Figs. 4, and 5, and 6.

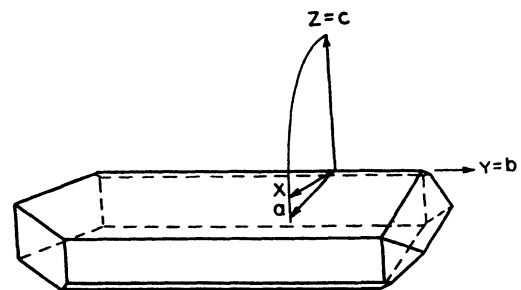


Fig. 5—Ethylene diamine d -tartrate (EDT), a monoclinic crystal, class 2. On extension along the b axis, the $+b$ end becomes positively charged.

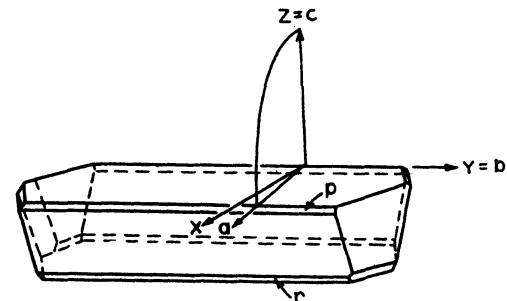


Fig. 6—Dipotassium d -tartrate (DKT), a monoclinic crystal, class 2. On extension along the b axis, the $+b$ end becomes positively charged.

1.5. The Orthorhombic System

Crystals having three mutually perpendicular two-fold axes or two mutually perpendicular planes of reflection symmetry, or both, belong to the orthorhombic

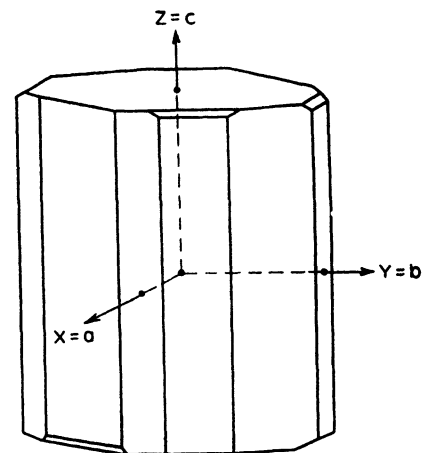


Fig. 7—Rochelle salt, an orthorhombic crystal, class 2 2 2.