



Physical Properties

Reading Assignment:

1. J. F. Nye, Physical Properties of Crystals
2. R. E. Newnham, Properties of Materials
3. R. E. Newnham, Structure–property Relations





Contents



- 1** Physical Properties
- 2** First Rank Tensor
- 3** Second Rank Tensor
- 4** Third Rank Tensor
- 5** Fourth Rank Tensor





Physical Properties of Crystals



- first rank tensor
- pyroelectricity: develop an electric polarization when their temperature is changed

$$\Delta P_i = p_i \Delta T \quad (p_i : \text{pyroelectric coefficient})$$

- hydrostatic pressure instead of temperature change
- experiment- clamped- primary pyroelectricity
free - secondary pyroelectricity





Pyroelectricity



- Neumann's principle

in a crystal possessing a center of symmetry

$$\vec{p} = 0$$

inversion center $p_1 \rightarrow -p_1, p_2 \rightarrow -p_2, p_3 \rightarrow -p_3$

property is unchanged after applying the symmetry

element $p_1 \rightarrow -p_1 = p_1 \quad p_1 = 0$

centrosymmetric (11 groups) \rightarrow non-pyroelectric

$$\bar{1}, \frac{2}{m}, \frac{2}{m} \frac{2}{m} \frac{2}{m}, \bar{3}, \bar{3} \frac{2}{m}, \frac{4}{m}, \frac{4}{m} \frac{2}{m} \frac{2}{m}$$

$$\frac{6}{m}, \frac{6}{m} \frac{2}{m} \frac{2}{m}, \frac{2}{m} \bar{3}, \frac{4}{m} \bar{3} \frac{2}{m}$$





Pyroelectricity



- a pyroelectric moment can only lie along a direction in a crystal which is **unique**, in the sense that it is not repeated by any symmetry element.
- polar direction: 이 축에 수직인 2회 회전축이나 거울면을 갖지 않는 극성을 갖는 축
ex) point group 32
a diad axis is a polar, but not unique direction
- all unique directions are polar, but only some polar directions are unique.





Pyroelectricity



Triclinic

Class 1: no symmetry restriction on the direction of \mathbf{p} : (p_1, p_2, p_3) .

Monoclinic. x_2 parallel to the diad axis, rotation or inverse, (y) .

Class 2: \mathbf{p} parallel to the diad axis: $(0, p, 0)$.

Class m : \mathbf{p} has any direction in the symmetry plane: $(p_1, 0, p_3)$.

Orthorhombic. x_1, x_2, x_3 parallel to crystallographic x, y, z respectively.

Class $mm2$: \mathbf{p} parallel to the diad axis: $(0, 0, p)$.

Class 222 : $(0, 0, 0)$.

Tetragonal, trigonal, hexagonal. x_3 parallel to z .

Classes $4, 4mm, 3, 3m, 6, 6mm$: \mathbf{p} parallel to the 4, 3 or 6 axis: $(0, 0, p)$.

Classes $\bar{4}, \bar{4}2m, \bar{4}22, 32, \bar{6}, \bar{6}m2, 622$: $(0, 0, 0)$.

Cubic

Classes $432, \bar{4}3m, 23$: $(0, 0, 0)$.





Pyroelectricity



- polar class- non-zero pyroelectric coefficients

1, 2, 3, 4, 6, m , $2mm$, $3m$, $4mm$, $6mm$

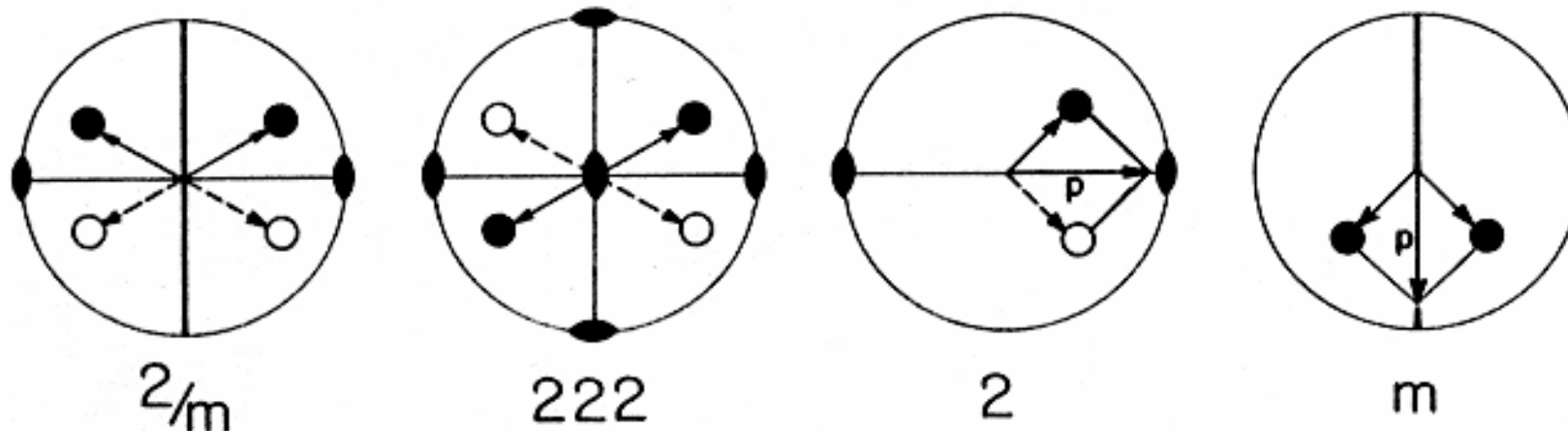


Fig. 31. Dipole configurations in two monoclinic and two orthorhombic point groups. In centric point groups like $2/m$, every dipole is cancelled by an equal and opposite dipole. These point groups are neither pyroelectric nor piezoelectric. Dipole cancellation also occurs in certain acentric point groups such as 222 . These point groups are generally piezoelectric but not pyroelectric. Dipoles do not cancel in point groups 2 and m which are both piezoelectric and pyroelectric. In 2 , the net spontaneous polarization must lie along the rotation axis. In m , P_s lies somewhere in the mirror plane





Pyroelectricity



-Wurtzite-hexagonal ZnS-6mm
polar axis and P are parallel to c, six-fold axis

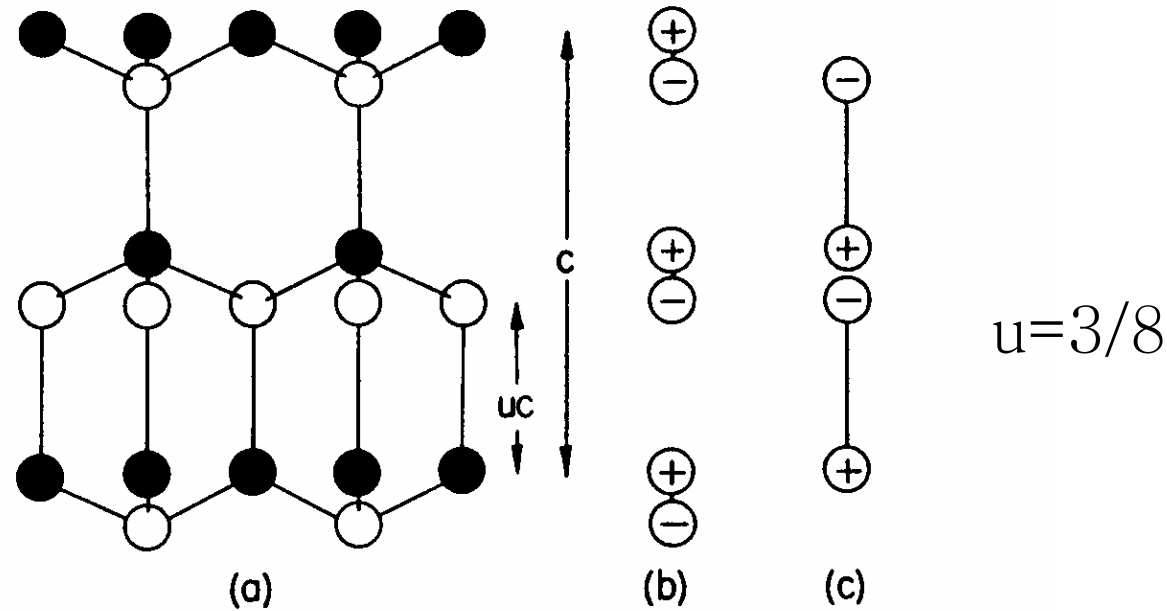


Fig. 32a-c. Wurtzite structure projected on (010), and equivalent polar chains showing two ways in which the crystal can terminate

$$p = + (1/2 - u)c \quad p = -quc$$





Pyroelectricity

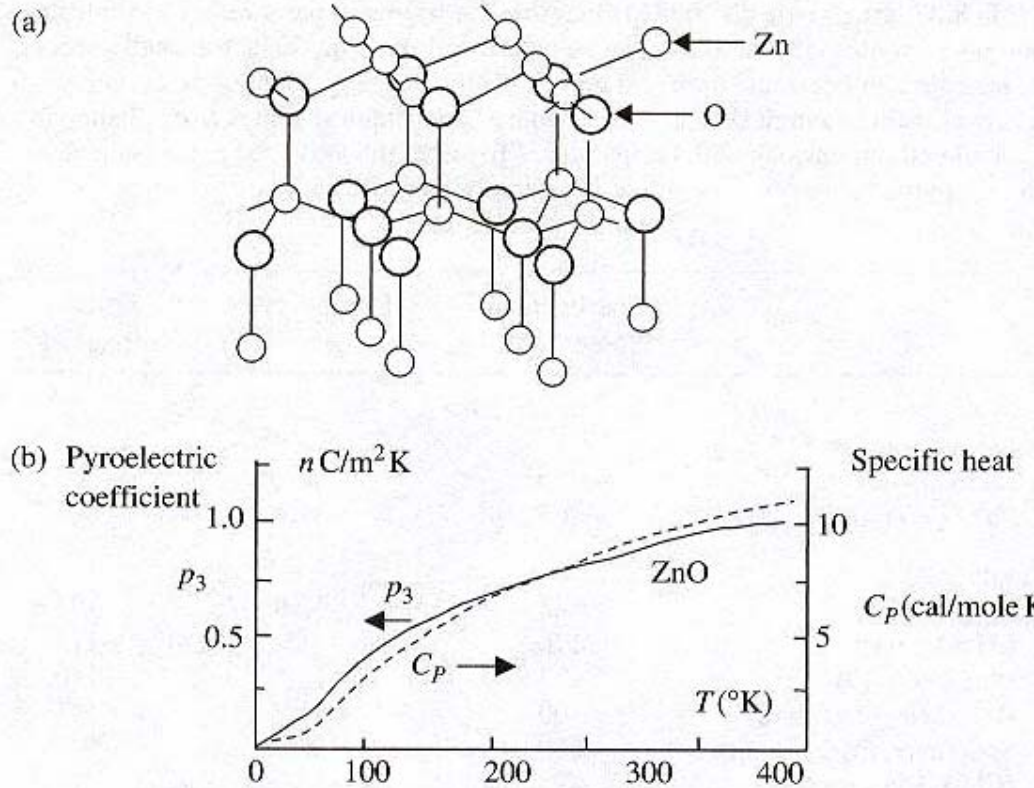


Fig. 8.4 (a) Crystal structure of zinc oxide showing the polar orientation of the zinc-oxygen bonds along the hexagonal c -axis. ZnO has the wurtzite structure and belongs to polar group $6mm$. (b) The pyroelectric coefficients of nonferroelectric crystals are generally small and correlate well with specific heat.

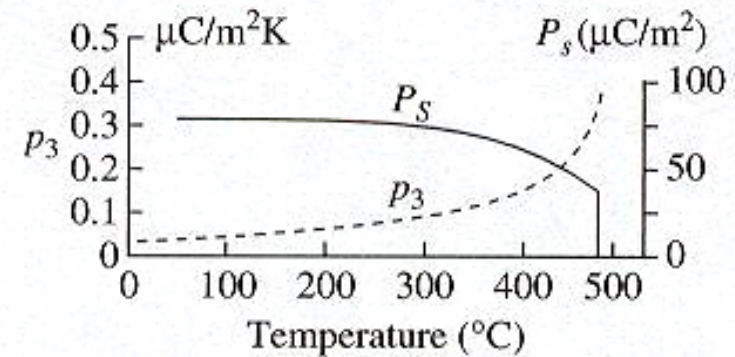
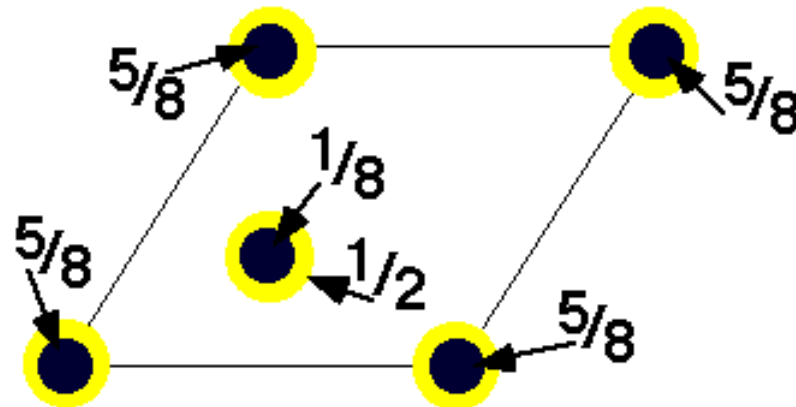
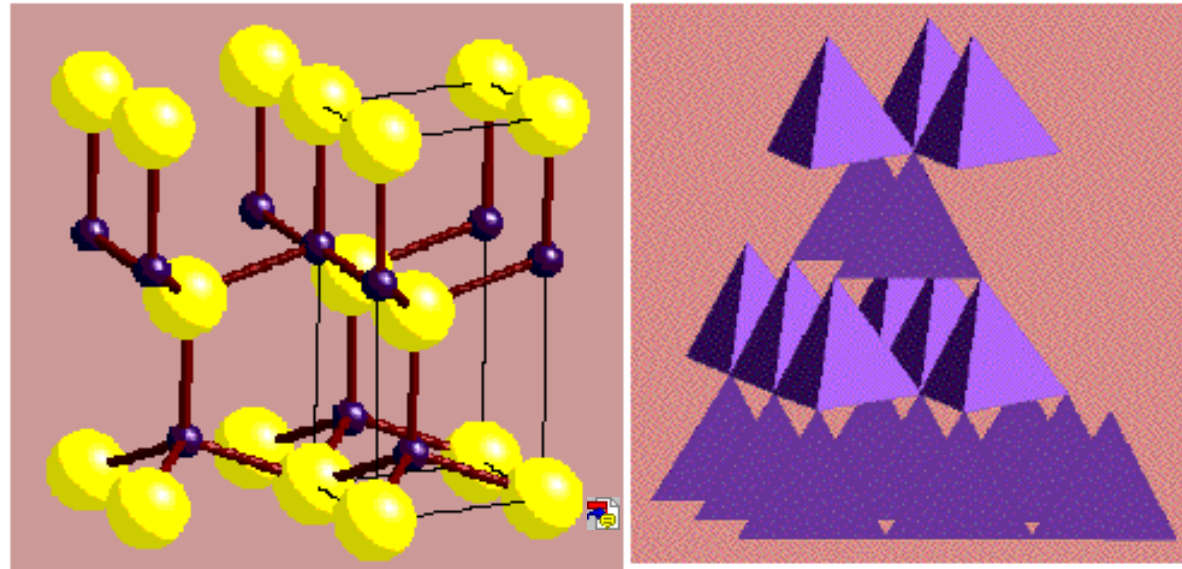


Fig. 8.5 In poled ferroelectric crystals the pyroelectric effect is the temperature derivative of the spontaneous polarization. PbTiO_3 polarizes along the tetragonal c -axis. Both P_s and the pyroelectric coefficient p_3 are zero above T_c where the symmetry changes to cubic at 490°C .





ZnS *Wurtzite*



http://www.chem.ox.ac.uk/icl/heyes/structure_of_solids/Strucsol.html





ZnS *Wurtzite*



- HCP S^{2-} with Zn^{2+} in half Tetrahedral holes (only T^+ {or T^- } filled)
- *Lattice*: Hexagonal - P
- $a = b, c \text{ \AA} \approx (8/3)a$
- *Motif*: 2S at $(0,0,0)$ & $(\frac{2}{3}, \frac{1}{3}, \frac{1}{2})$; 2Zn at $(\frac{2}{3}, \frac{1}{3}, \frac{1}{8})$ & $(0,0, \frac{5}{8})$
- 2ZnS in unit cell
- *Coordination*: 4:4 (tetrahedral)

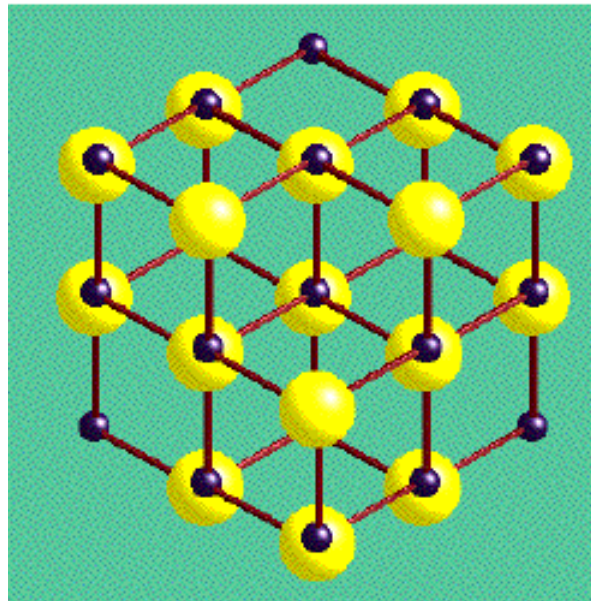




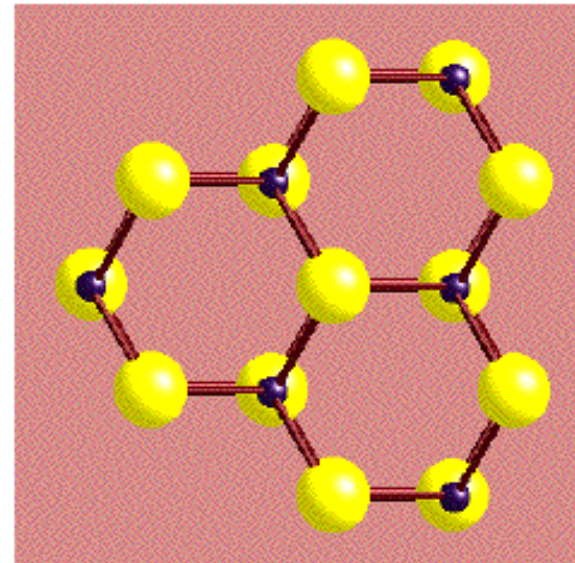
Comparison of Wurtzite and Zinc Blende



PLAN VIEWS



Zinc Blende
CCP ABC repeat



Wurtzite
HCP AB repeat

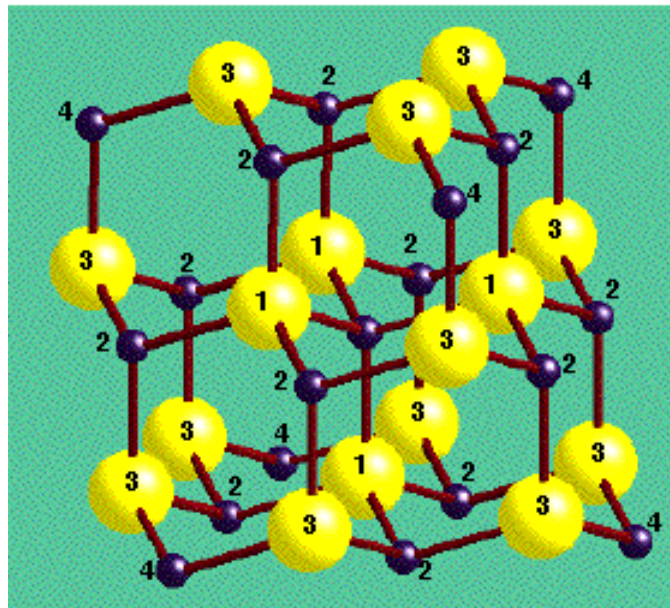




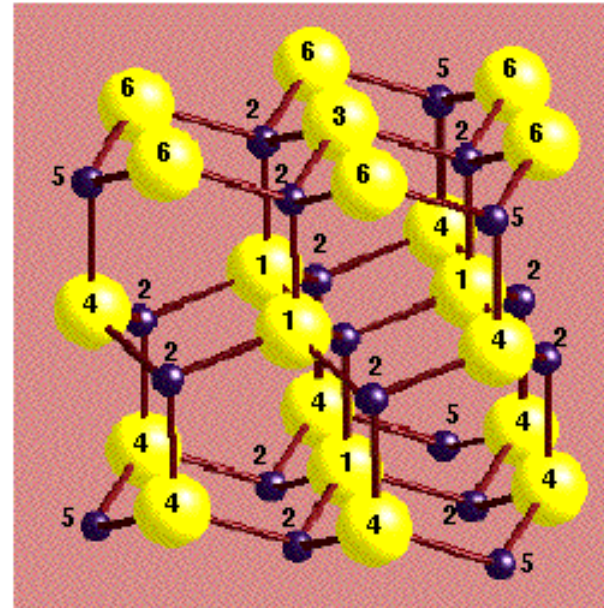
Comparison of Wurtzite and Zinc Blende



COORDINATION ENVIRONMENTS



Zinc Blende



Wurtzite

4 Nearest Neighbours (*Tetrahedral*)

12 Next-Nearest Neighbours

Cuboctahedral ←

→ *Anti-Cuboctahedral*

Very different Next, Next-Nearest Neighbour Coordinations & beyond

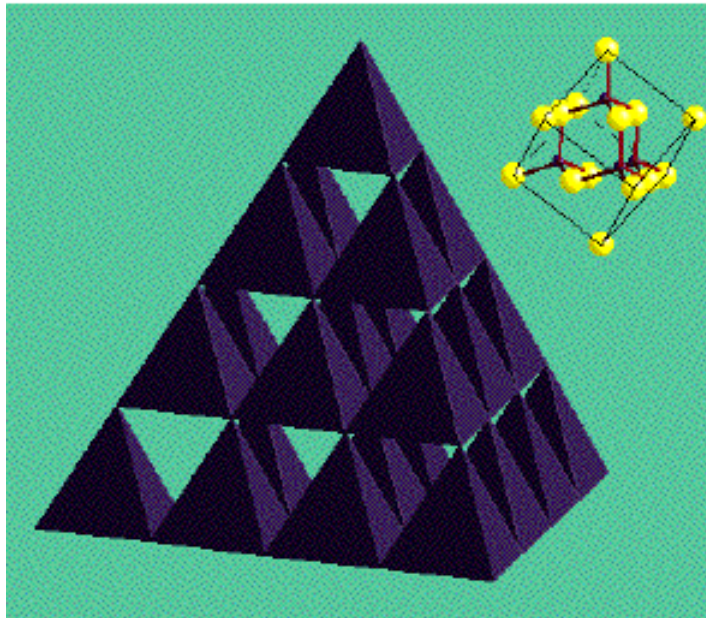




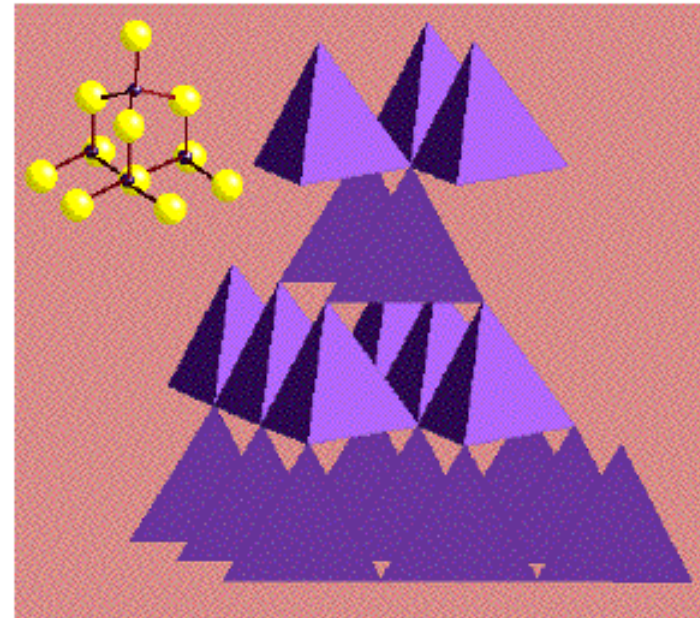
Comparison of Wurtzite and Zinc Blende



POLYHEDRAL REPRESENTATIONS



Zinc Blende



Wurtzite

Vertex-linked tetrahedra only, but layers skewed in Wurtzite, & not in Blende





Pyroelectricity



Table 10. Comparison of pyroelectric detector materials [3]

Material	Operating temperature (°C)	Dielectric constant	Pyroelectric coefficient ($\times 10^{-7} \text{ C/}^\circ - \text{cm}^2$)	Figure of merit ($\times 10^{-11}$)
Triglycine sulfate	40	35	1.3	300
Lithium sulfate	25	10.3	0.078	76
Rochelle salt	22	1000	0.2	2
Barium titanate	25	4100	0.6	1.5
Lead zirconate titanate	25	2200	0.6	3

*used as infrared radiation detectors

- ferroelectricity: spontaneous polarization
reversability
hysteresis





Second Rank Tensor



– **electrical conductivity**

– Ohm's law

$$j_i = -\sigma_{ik} \frac{\partial \phi}{\partial x_k} = \sigma_{ik} E_k$$

where j_i : current density, σ_{ik} : electrical conductivity tensor

ϕ : potential, E_k : electric field intensity

$$E_i = \rho_{ik} j_k$$

Electrical resistivities of metallic crystals

Values of principal resistivities at 20° C (unit = 10⁻⁸ ohm-m)

<i>Crystal</i>	<i>System</i>	ρ_1, ρ_2	ρ_3
Tin	tetragonal	9.9	14.3
Bismuth	trigonal	109	138
Cadmium	hexagonal	6.80	8.30
Zinc	„	5.91	6.13
Tungsten	cubic	5.48	
Copper	„	1.51	



The effect of crystal symmetry on properties represented by symmetrical second-rank tensors

Optical classification	System	Characteristic symmetry (see p. 280)†	Nature of representation quadric and its orientation	Number of independent coefficients	Tensor referred to axes in the conventional orientation‡
Isotropic (anaxial)	Cubic	4 3-fold axes	Sphere	1	$\begin{bmatrix} S & 0 & 0 \\ 0 & S & 0 \\ 0 & 0 & S \end{bmatrix}$
Uniaxial	Tetragonal	1 4-fold axis	Quadric of revolution about the principal symmetry axis (x_3)(z)	2	$\begin{bmatrix} S_1 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_3 \end{bmatrix}$
	Hexagonal	1 6-fold axis			
	Trigonal	1 3-fold axis			
Biaxial	Orthorhombic	3 mutually perpendicular 2-fold axes; no axes of higher order	General quadric with axes (x_1, x_2, x_3) to the diad axes (x, y, z)	3	$\begin{bmatrix} S_1 & 0 & 0 \\ 0 & S_2 & 0 \\ 0 & 0 & S_3 \end{bmatrix}$
	Monoclinic	1 2-fold axis	General quadric with one axis (x_2) to the diad axis (y)	4	$\begin{bmatrix} S_{11} & 0 & S_{31} \\ 0 & S_2 & 0 \\ S_{31} & 0 & S_{33} \end{bmatrix}$
	Triclinic	A centre of symmetry or no symmetry	General quadric. No fixed relation to crystallographic axes	6	$\begin{bmatrix} S_{11} & S_{12} & S_{31} \\ S_{12} & S_{22} & S_{32} \\ S_{31} & S_{32} & S_{33} \end{bmatrix}$



Second Rank Tensor



- **thermal conductivity**

$$h_i = -K_{ij} \frac{\partial T}{\partial x_j}$$

where h_i : heat flow rate per unit area, K_{ij} : thermal conductivity tensor, $\frac{\partial T}{\partial x_j}$: temperature gradient

Thermal conductivities of crystals

Values of the principal conductivities in m.k.s. units [joule/(m sec °C)]

<i>Crystal</i>	<i>System</i>	<i>Temperature</i> °C	k_1, k_2	k_3
Quartz . .	trigonal	30	6.5	11.3
Calcite . .	„	30	4.18	4.98
Bismuth . .	„	18	9.24	6.65
Graphite . .	hexagonal	30	355	89
Aluminium . .	cubic	30	208	
Copper . .	„	0	410	





Second Rank Tensor



– electric polarization

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P}$$

where D : electric displacement, ϵ_0 : permittivity of vacuum

P : polarization

$$P_i = \epsilon_0 \chi_{ij} E_j \quad (\chi_{ij} : \text{dielectric susceptibility})$$

$$D_i = \epsilon_{ij} E_j, \quad \epsilon_{ij} = \epsilon_0 (\delta_{ij} + \chi_{ij})$$

relative dielectric constant

$$\epsilon_{rij} = \epsilon_{ij} / \epsilon_0$$





Second Rank Tensor



Dielectric constants of crystals

<i>Crystal</i>	<i>System</i>	K_1	K_2	K_3	<i>Frequency (cycles/sec.)</i>
Gypsum . . .	monoclinic	9.9	5.1	5.0	3×10^8
Aragonite . . .	orthorhombic	9.8	7.7	6.6	4×10^8
Quartz . . .	trigonal	4.5		4.6	50 to 5×10^8
Calcite . . .	„	8.5		8.0	4×10^8
Rutile . . .	tetragonal	89		173	4×10^8
Caesium chloride	cubic	6.3			2×10^5
Sodium chloride	„	5.6			2×10^5





Second Rank Tensor



– magnetization

$$\vec{B} = \mu_o \vec{H} + \mu_o \vec{M}$$

where D : magnetic induction, μ_o : permeability of vacuum

M : magnetization

$$M_i = \chi_{mij} H_j \quad (\chi_{mij} : \text{magnetic susceptibility})$$

$$B_i = \mu_{ij} H_j, \quad \mu_{ij} = \mu_o (\delta_{ij} + \chi_{mij})$$

relative permeability

$$\mu_{rij} = \mu_{ij} / \mu_o$$





Second Rank Tensor



Susceptibilities of paramagnetic and diamagnetic crystals

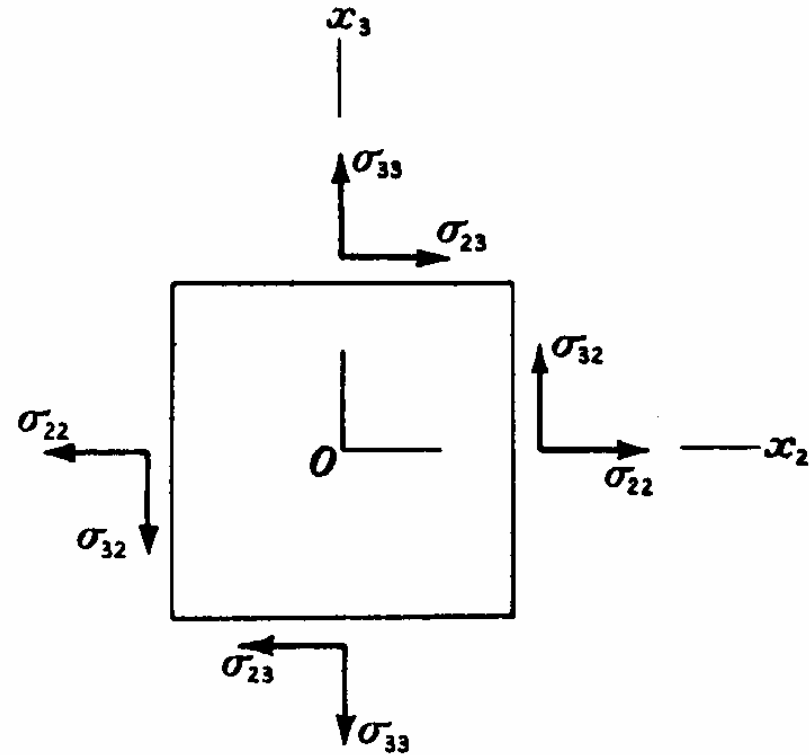
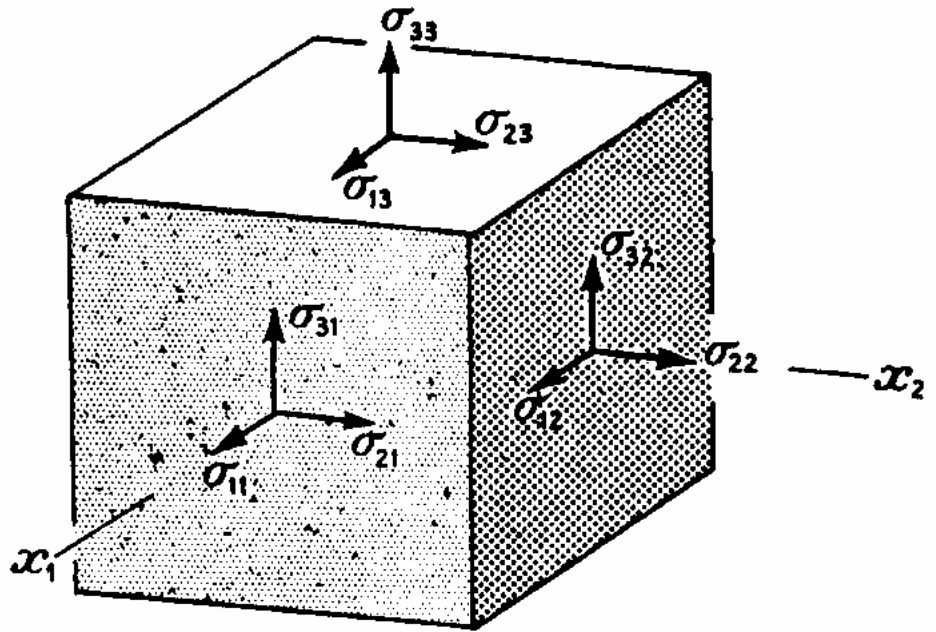
When multiplied by 10^{-6} the numbers in the table are the volume susceptibilities in rationalized units.

<i>Crystal</i>	<i>System</i>	ψ_1	ψ_2	ψ_3	<i>Ref.</i>
Aragonite .	orthorhombic	-1.44	-1.42	-1.63	1
Quartz . .	trigonal	-1.51		-1.52	2
Calcite . .	„	-1.24		-1.38	1
Cadmium . .	hexagonal	-1.74		-2.85	3
Beryl . .	„	2.76		1.29	1
Rutile . .	tetragonal	10.5		11.2	1
Fluorite . .	cubic		-1.14		1
Sodium chloride	„		-1.36		1





Stress and Strain



$$\begin{bmatrix} \sigma_{11} & \sigma_{21} & \sigma_{31} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}$$

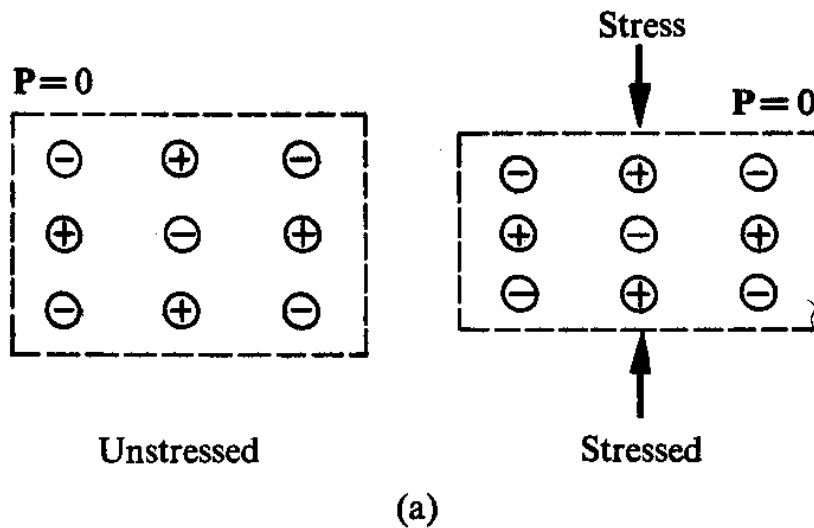




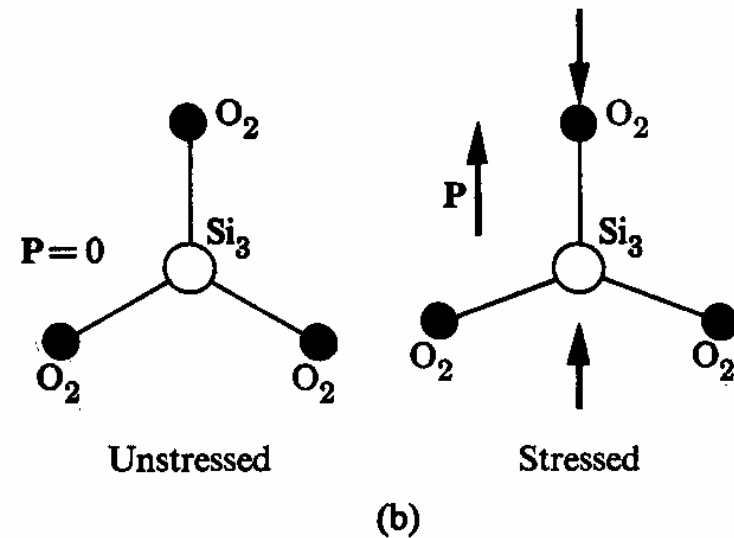
Third Rank Tensor



- piezoelectricity
 - direct piezoelectric effect
stress \rightarrow electric dipole moment
- $$P = d\sigma \quad (\text{piezoelectric modulus})$$



inversion center



quartz





Third Rank Tensor

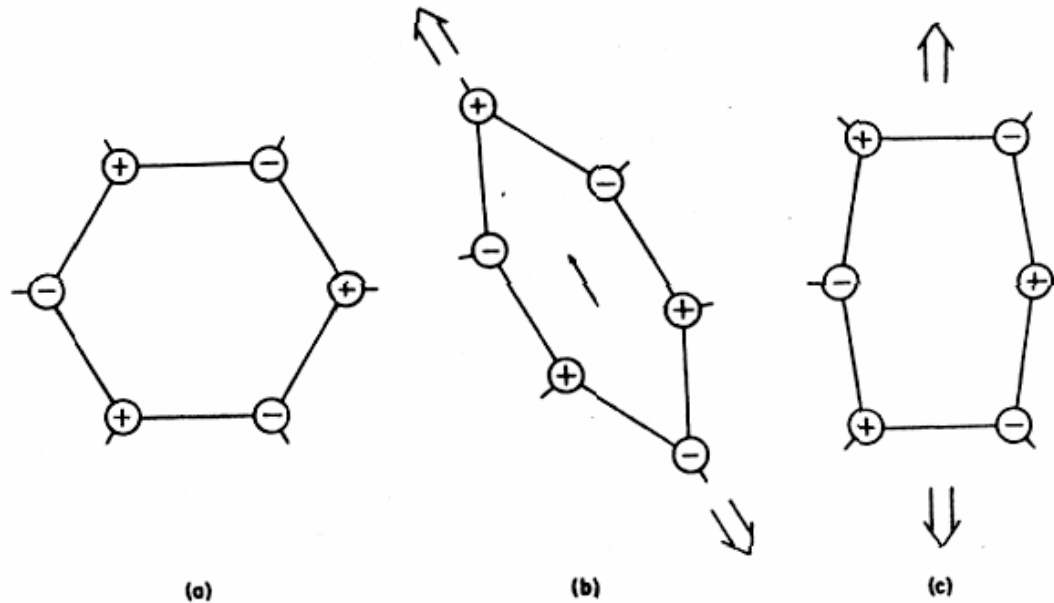


Fig. 33a-c. Unstressed (a) and stressed (b,c) structures containing positive and negative ions. Polarization, a separation of positive and negative charge centers, is achieved in (b) but not in (c), showing that not all directions are piezoelectric

Some Piezoelectric Crystals (in Decreasing Value of Piezoelectric Coefficient)

Crystal	Chemical formula	Relative strength
Rochelle salt	$\text{NaKC}_4\text{H}_4\text{O}_6 \cdot 4\text{H}_2\text{O}$	Very strong
ADP	$\text{NH}_4\text{H}_2\text{PO}_4$	Strong
KDP	KH_2PO_4	Moderate
α -Quartz	SiO_2	Weak





Third Rank Tensor



- $P_i = d_{ijk} \sigma_{jk}$

- $P_1 = d_{111} \sigma_{11} + d_{112} \sigma_{12} + d_{113} \sigma_{13} + d_{121} \sigma_{21} + d_{122} \sigma_{22} + d_{123} \sigma_{23}$
 $+ d_{131} \sigma_{31} + d_{132} \sigma_{32} + d_{133} \sigma_{33}$

- d_{ijk} : 27 coefficients

- third rank tensor: $d_{ijk} = a_{il} a_{jm} a_{kn} d_{lmn}$





Third Rank Tensor



1st layer

$$i = 1$$

$$d_{111} \quad d_{112} \quad d_{113}$$

$$(d_{121}) \quad d_{122} \quad d_{123}$$

$$(d_{131})(d_{132}) \quad d_{133}$$

2nd layer

$$i = 2$$

$$d_{211} \quad d_{212} \quad d_{213}$$

$$(d_{221}) \quad d_{222} \quad d_{223}$$

$$(d_{231})(d_{232}) \quad d_{233}$$

3rd layer

$$i = 3$$

$$d_{311} \quad d_{312} \quad d_{313}$$

$$(d_{321}) \quad d_{322} \quad d_{323}$$

$$(d_{331})(d_{332}) \quad d_{333}$$

- $d_{ijk} = d_{ikj}$ (18 independent components)

- matrix notation

$$d_{11} \quad \frac{1}{2} d_{16} \quad \frac{1}{2} d_{15}$$

$$d_{12} \quad \frac{1}{2} d_{14}$$

$$d_{13}$$

$$d_{21} \quad \frac{1}{2} d_{26} \quad \frac{1}{2} d_{25}$$

$$d_{22} \quad \frac{1}{2} d_{24}$$

$$d_{23}$$

$$d_{31} \quad \frac{1}{2} d_{36} \quad \frac{1}{2} d_{35}$$

$$d_{32} \quad \frac{1}{2} d_{34}$$

$$d_{33}$$





Third Rank Tensor



- tensor notation: 11 22 33 23,32 31,13, 12,21

matrix notation: 1 2 3 4 5 6

$$- \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \rightarrow \begin{bmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \sigma_6 & \sigma_2 & \sigma_4 \\ \sigma_5 & \sigma_4 & \sigma_3 \end{bmatrix}$$

$$- P_1 = d_{11}\sigma_1 + \frac{1}{2}d_{16}\sigma_6 + \frac{1}{2}d_{15}\sigma_5 + \frac{1}{2}d_{16}\sigma_6 + d_{12}\sigma_2 + \frac{1}{2}d_{14}\sigma_4 \\ + \frac{1}{2}d_{15}\sigma_5 + \frac{1}{2}d_{14}\sigma_4 + d_{13}\sigma_3$$

$$= d_{11}\sigma_1 + d_{12}\sigma_2 + d_{13}\sigma_3 + d_{14}\sigma_4 + d_{15}\sigma_5 + d_{16}\sigma_6$$

$$- p_i = d_{ij}\sigma_j \quad (i = 1, 2, 3, j = 1, 2, \dots, 6)$$





Third Rank Tensor



- array of d_{ij}

$$\begin{pmatrix} d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\ d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\ d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36} \end{pmatrix}$$

- the d_{ij} do not transform like the components of a second rank tensor

- converse piezoelectric effect

electric field \rightarrow strain

$$\varepsilon_{jk} = d_{ijk} E_i$$

(matrix notation: $\varepsilon_j = d_{ij} E_i (i = 1, 2, 3, j = 1, 2, \dots, 6)$)





Third Rank Tensor



$$\begin{array}{c}
 \begin{array}{c} \downarrow \\ E_1 \\ E_2 \\ E_3 \end{array} \\
 \begin{array}{c} \rightarrow \\ P_1 \\ P_2 \\ P_3 \end{array}
 \end{array}
 \begin{array}{c}
 \begin{array}{cccccc}
 \epsilon_1 & \epsilon_2 & \epsilon_3 & \epsilon_4 & \epsilon_5 & \epsilon_6 \\
 \sigma_1 & \sigma_2 & \sigma_3 & \sigma_4 & \sigma_5 & \sigma_6
 \end{array} \\
 \left[\begin{array}{cccccc}
 d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\
 d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\
 d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36}
 \end{array} \right]
 \end{array}$$

Defining equations for the direct and converse piezoelectric effects

	<i>Tensor notation</i> ($i, j, k = 1, 2, 3$)	<i>Matrix notation</i> ($i = 1, 2, 3; j = 1, 2, \dots, 6$)
Direct effect . . .	$P_i = d_{ijk} \sigma_{jk}$	$P_i = d_{ij} \sigma_j$
Converse effect . . .	$\epsilon_{jk} = d_{ijk} E_i$	$\epsilon_j = d_{ij} E_i$

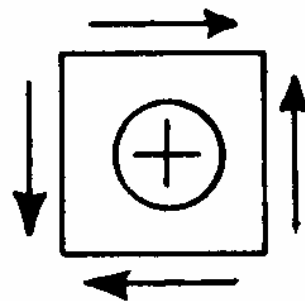
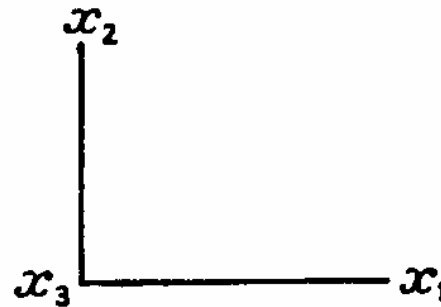




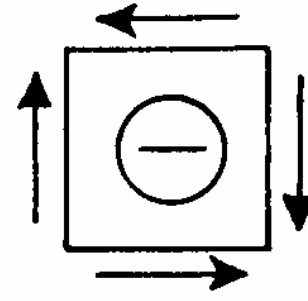
Third Rank Tensor



- reduction in the number of independent moduli by crystal symmetry
- a crystal with a center of symmetry cannot be piezoelectric
- modulus d_{36} in class 4



a



b

$$d_{36} = 0$$

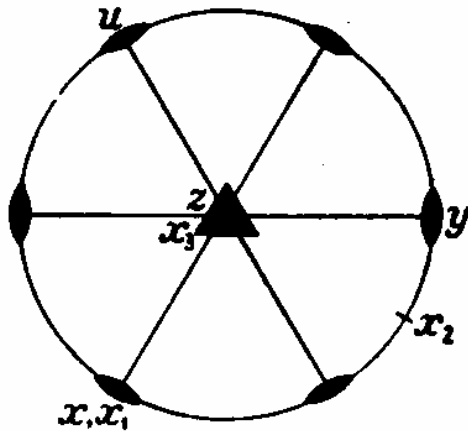




Third Rank Tensor



- piezoelectric: 20 point groups
(32 groups- centro-symmetric groups (11)-432)
- quartz (point group: 32)



$$\begin{matrix}
 P_1 \\
 P_2 \\
 P_3
 \end{matrix}
 \begin{matrix}
 \sigma_1 & \sigma_2 & \sigma_3 & \sigma_4 & \sigma_5 & \sigma_6
 \end{matrix}
 \begin{pmatrix}
 d_{11} & -d_{11} & 0 & d_{14} & 0 & 0 \\
 0 & 0 & 0 & 0 & -d_{14} & -2d_{11} \\
 0 & 0 & 0 & 0 & 0 & 0
 \end{pmatrix}$$

- tensile stress σ_1 parallel to x_1

$$P_1 = d_{11}\sigma_1, \quad P_2 = 0, \quad P_3 = 0$$

- tensile stress σ_2 parallel to x_2

$$P_1 = -d_{11}\sigma_1, \quad P_2 = 0, \quad P_3 = 0$$

$$\begin{pmatrix}
 -2.3 & 2.3 & 0 & -0.67 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0.67 & 4.6 \\
 0 & 0 & 0 & 0 & 0 & 0
 \end{pmatrix} \times 10^{-12} \text{ C/N}$$





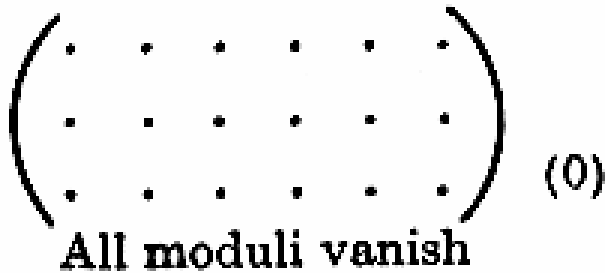
Third Rank Tensor



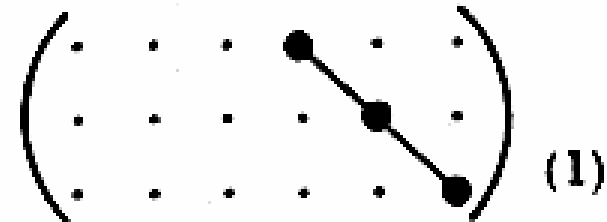
- zinc blende ZnS (point group: $\bar{4}3m$)

CUBIC

Class 432



Classes $\bar{4}3m$ and 23



$$-P_1 = d_{14}\sigma_4$$

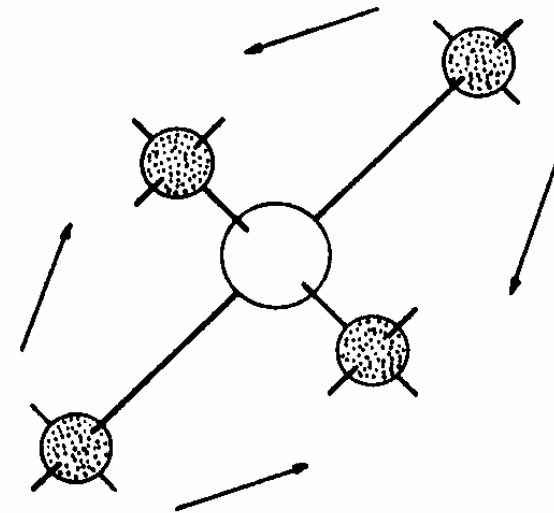
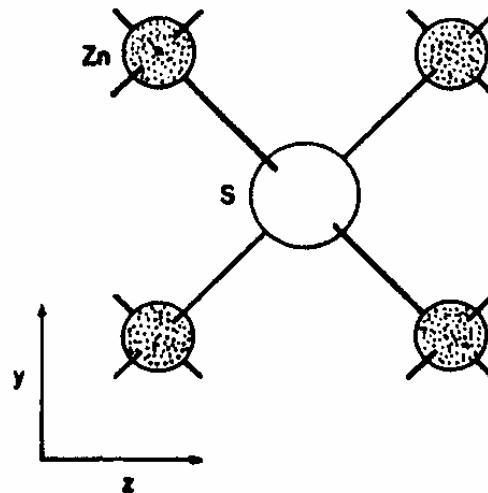
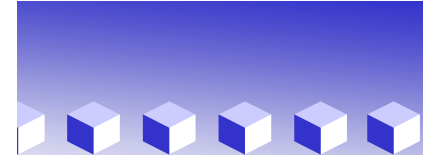


Fig. 35a and b. A single tetrahedron of the zincblende structure, unstressed (a) and under shear stress (b), viewed along the polarization direction





Form of the (d_{ij}) matrix

KEY TO NOTATION	
•	zero modulus
●	non-zero modulus
●—●	equal moduli
●—○	moduli numerically equal, but opposite in sign
⊙	a modulus equal to minus 2 times the heavy dot modulus to which it is joined.

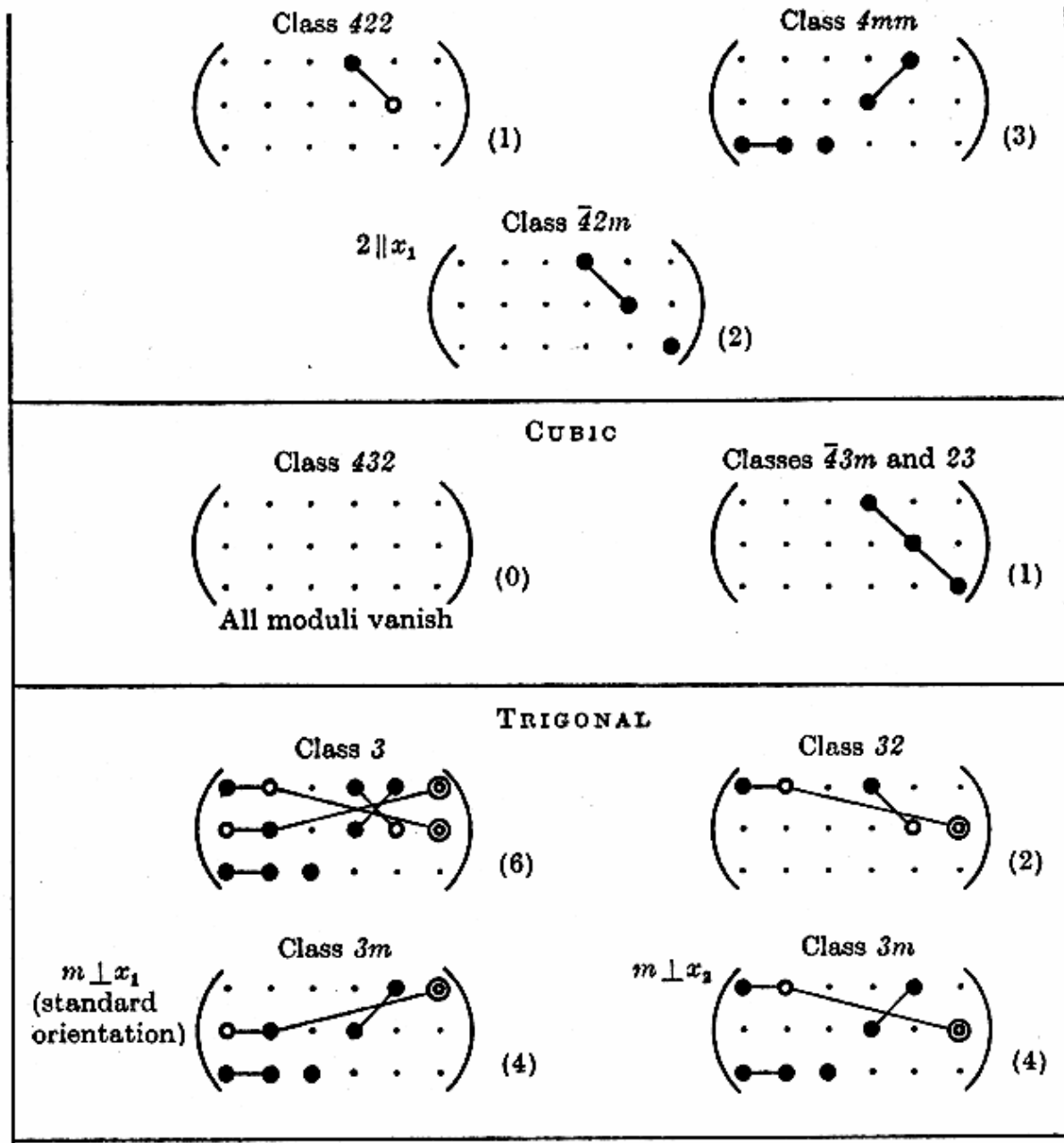
Centrosymmetrical classes

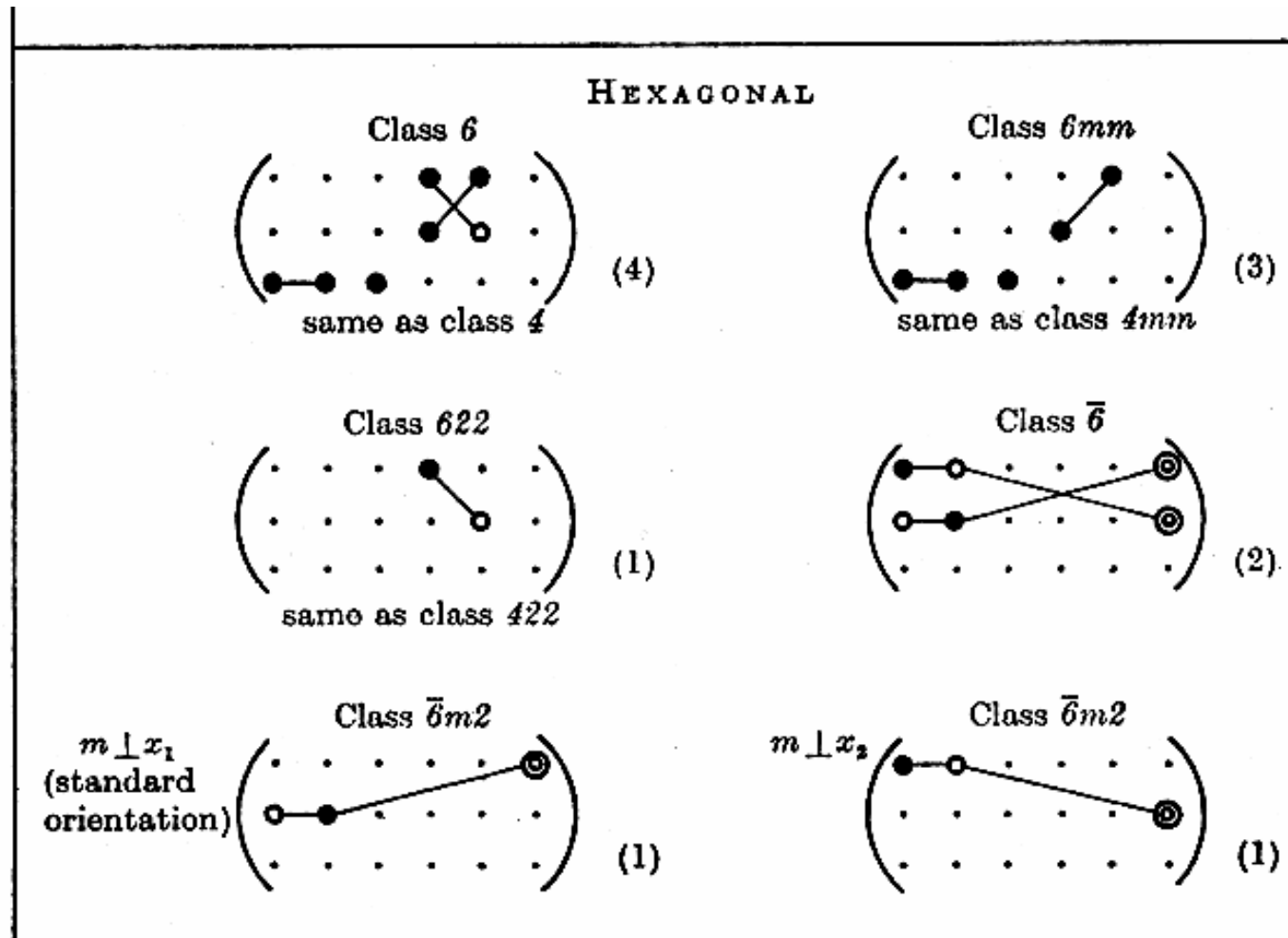
All moduli vanish

Non-centrosymmetrical classes

TRICLINIC Class 1 $\begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} (18)$		
MONOCLINIC Class 2 $2 \parallel x_3$ (standard orientation)	$\begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} (8)$	$2 \parallel x_3$ Class 2 $\begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} (8)$
$m \perp x_3$ (standard orientation)	Class m $\begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} (10)$	$m \perp x_3$ Class m $\begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} (10)$
ORTHORHOMBIC Class 222 $\begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} (3)$		Class mm2 $\begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} (5)$
TETRAGONAL Class 4 $\begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} (4)$		Class $\bar{4}$ $\begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} (4)$









Fourth Rank Tensor



- Hook's law

$$\sigma_{ij} = c_{ijkl} \varepsilon_{kl} \quad (c_{ijkl}: \text{stiffness, Young modulus})$$

$$\varepsilon_{ij} = s_{ijkl} \sigma_{kl} \quad (s_{ijkl}: \text{compliance})$$

- 81 components

$$c_{ijkl} = c_{ijlk}, \quad c_{ijkl} = c_{jikl} \quad (36 \text{ components})$$

- matrix notation

$$\sigma_i = c_{ij} \varepsilon_j \quad (i, j = 1, 2, \dots, 6)$$

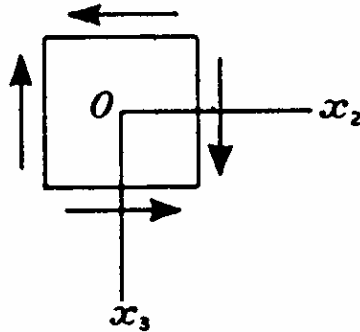
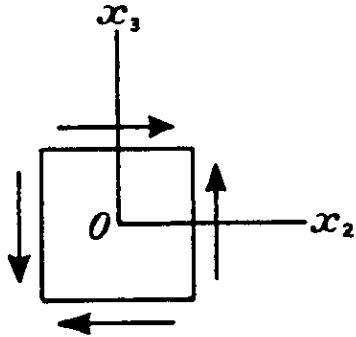
6x6 matrix

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{21} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{31} & c_{32} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{41} & c_{42} & c_{43} & c_{44} & c_{45} & c_{46} \\ c_{51} & c_{52} & c_{53} & c_{54} & c_{55} & c_{56} \\ c_{61} & c_{62} & c_{63} & c_{64} & c_{65} & c_{66} \end{pmatrix}$$



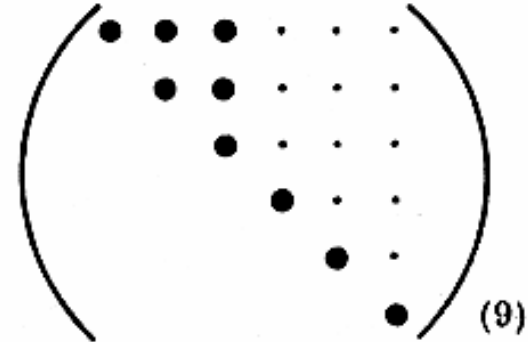
Fourth Rank Tensor

-orthorhombic class 222: s_{34}



ORTHORHOMBIC

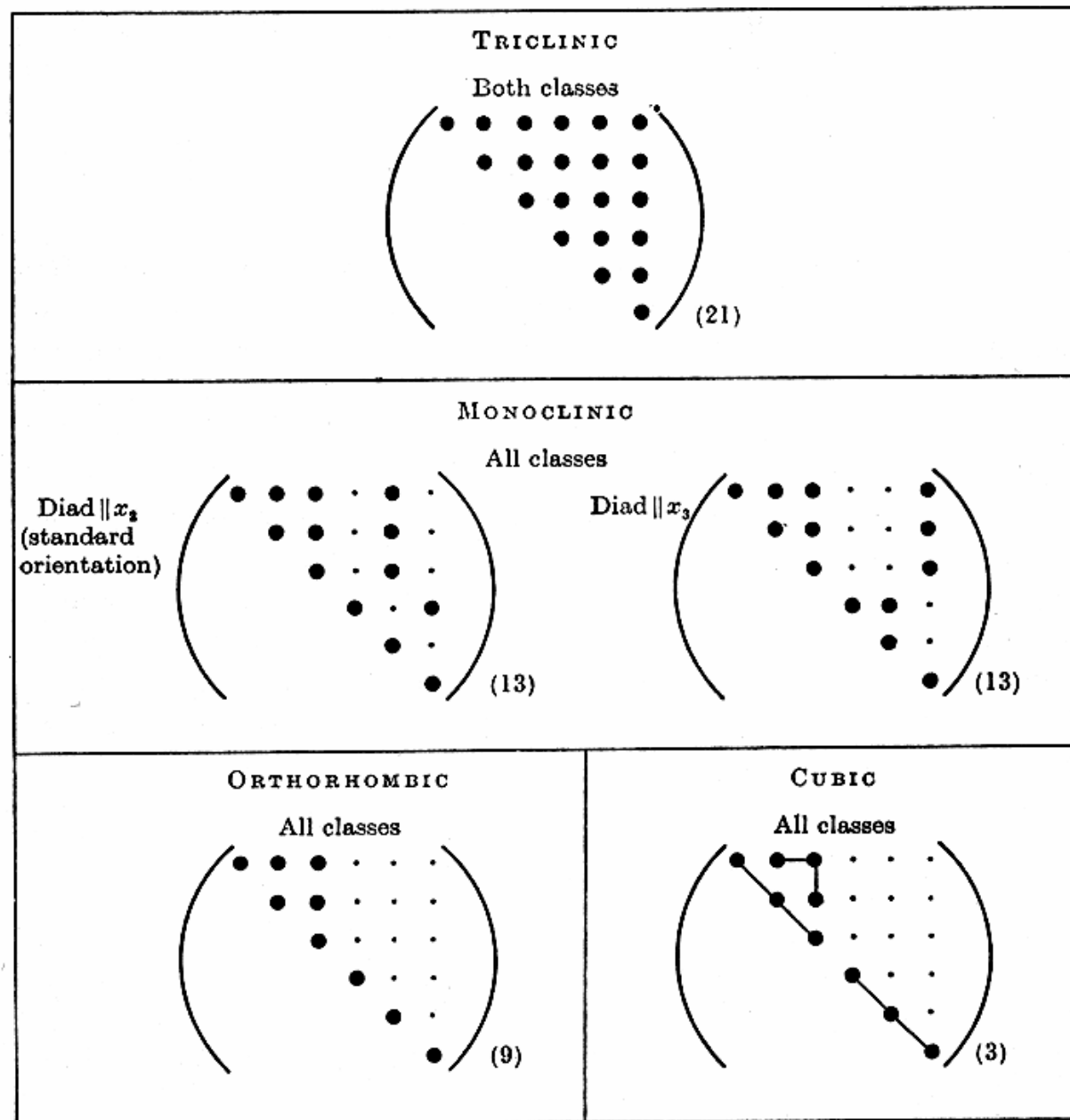
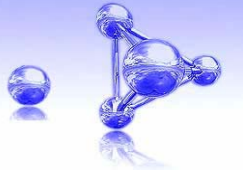
All classes



Elasticity of Crystals

Compliances at room temperature (unit = 10^{-11} m²/newton)

Crystal	Class	s_{11}	s_{12}	s_{44}	s_{33}	s_{13}	s_{14}	s_{66}
Sodium chloride	$m\bar{3}m$	2.21	-0.45	7.83
Aluminium	$m\bar{3}m$	1.59	-0.58	3.52
Copper	$m\bar{3}m$	1.49	-0.63	1.33
Nickel	$m\bar{3}m$	0.799	-0.312	0.844
Tungsten	$m\bar{3}m$	0.257	-0.073	0.660
Sodium chlorate	23	2.2	-0.6	8.6
Tin	$4/m\bar{3}m$	1.85	-0.99	5.70	1.18	-0.25	..	13.5
ADP	$42m$	1.8	0.7	11.3	4.3	-1.1	..	16.2
Zinc	$6/m\bar{3}m$	0.84	0.11	2.64	2.87	-0.78
Cadmium	$6/m\bar{3}m$	1.23	-0.15	5.40	3.55	-0.93
Quartz	32	1.27	-0.17	2.01	0.97	-0.15	-0.43	..
Tourmaline	$3m$	0.40	-0.10	1.51	0.63	-0.016	0.058	..



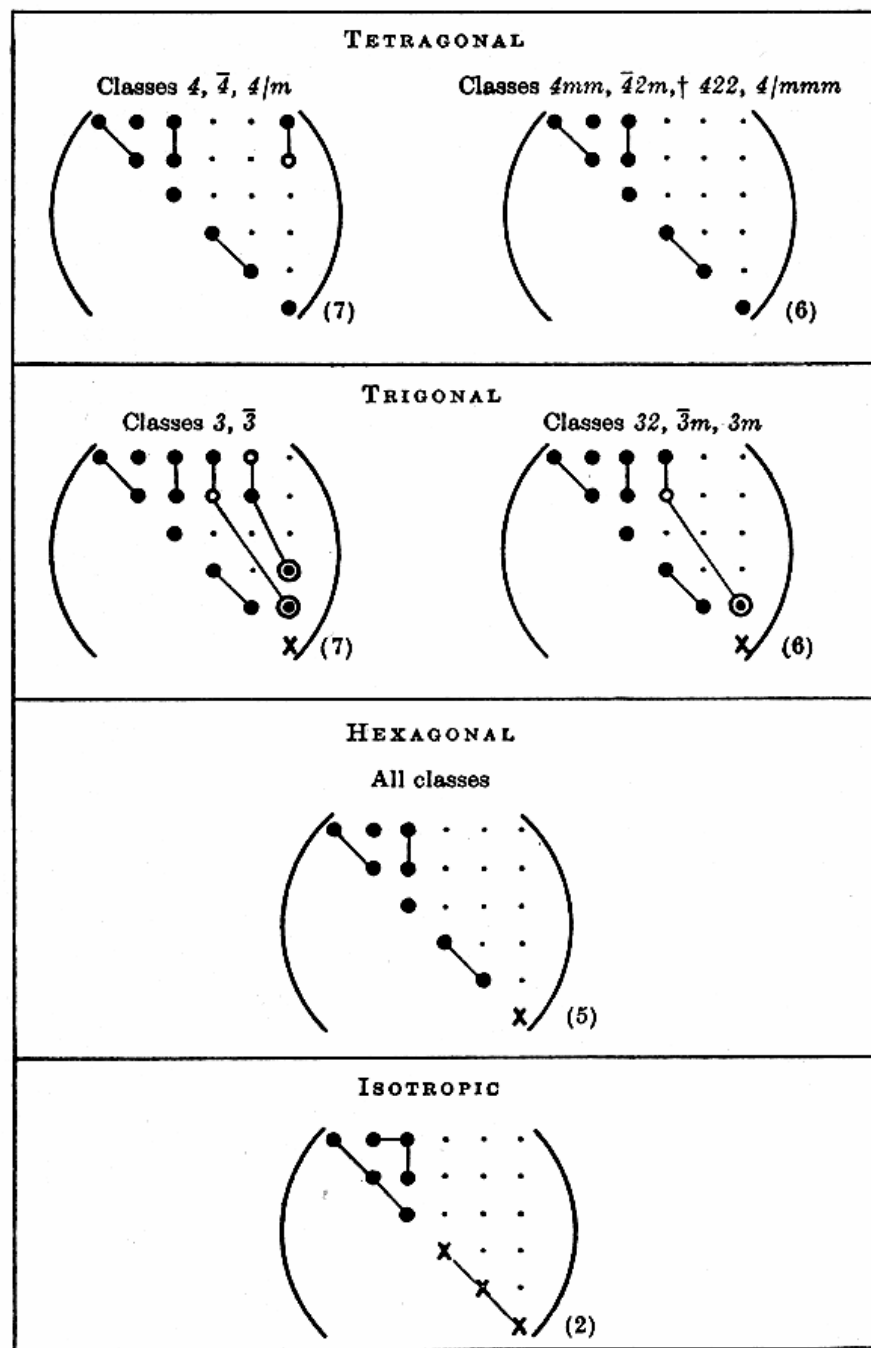
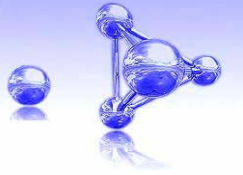
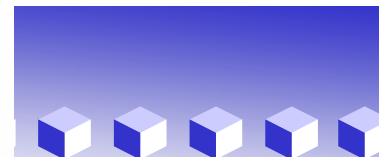




Table 4. Tensor properties for the 32 crystal classes [8]. Zero means the effect is absent. Other numbers indicate the number of non-zero coefficients, and the number of independent non-zero coefficients is given in parentheses. Third- and fourth-rank tensors are referred to the shortened two-subscript matrix notation



Crystal class	Tensor rank				Example
	1	2	3	4	
$1 = C_1$	3(3)	9(6)	18(18)	36(21)	Kaolinite $Al_2Si_2O_5(OH)$
$\bar{1} = C_i$	0	9(6)	0	36(21)	Copper sulfate $CuSO_4 \cdot 5H_2O$
$2 = C_2$	1(1)	5(4)	8(8)	20(13)	Sucrose $C_{12}H_{22}O_{11}$
$m = C_s$	2(2)	5(4)	10(10)	20(13)	Potassium nitrite KNO_2
$2/m = C_{2h}$	0	5(4)	0	20(13)	Orthoclase $KAlSi_3O_8$
$222 = D_2$	0	3(3)	3(3)	12(9)	Iodic acid HIO_3
$mm2 = C_{2v}$	1(1)	3(3)	5(5)	12(9)	Sodium nitrite $NaNO_2$
$mmm = D_{2h}$	0	3(3)	0	12(9)	Forsterite Mg_2SiO_4
$3 = C_3$	1(1)	3(2)	13(6)	24(7)	Nickel tellurate Ni_3TeO_6
$\bar{3} = C_{3i}$	0	3(2)	0	24(7)	Ilmenite $FeTiO_3$
$32 = D_3$	0	3(2)	5(2)	18(6)	Low-quartz SiO_2
$3m = C_{3v}$	1(1)	3(2)	8(4)	18(6)	Lithium niobate $LiNbO_3$
$\bar{3}m = D_{3d}$	0	3(2)	0	18(6)	Corundum Al_2O_3
$4 = C_4$	1(1)	3(2)	7(4)	16(7)	Iodosuccinimide $C_4H_4INO_2$
$\bar{4} = S_4$	0	3(2)	7(4)	16(7)	Boron phosphate BPO_4
$4/m = C_{4h}$	0	3(2)	0	16(7)	Scheelite $CaWO_4$
$422 = D_4$	0	3(2)	2(1)	12(6)	Nickel sulfate $NiSO_4 \cdot 6H_2O$
$4mm = C_{4v}$	1(1)	3(2)	5(3)	12(6)	Barium titanate $BaTiO_3$
$\bar{4}2m = D_{2d}$	0	3(2)	3(2)	12(6)	Potassium dihydrogen phosphate KH_2PO_4
$4/mmm = D_{4h}$	0	3(2)	0	12(6)	Rutile TiO_2
$6 = C_6$	1(1)	3(2)	7(4)	12(5)	Nepheline $NaAlSi_3O_8$
$\bar{6} = C_{3h}$	0	3(2)	6(2)	12(5)	Lead germanate $Pb_5Ge_3O_{11}$
$6/m = C_{6h}$	0	3(2)	0	12(5)	Apatite $Ca_5(PO_4)_3F$
$622 = D_6$	0	3(2)	2(1)	12(5)	High-quartz SiO_2
$6mm = C_{6v}$	1(1)	3(2)	5(3)	12(5)	Zincite ZnO
$\bar{6}m2 = D_{3h}$	0	3(2)	3(1)	12(5)	Benitoite $BaTiSi_3O_9$
$6/mmm = D_{6h}$	0	3(2)	0	12(5)	Beryl $Be_3Al_2Si_6O_{18}$
$23 = T$	0	3(1)	3(1)	12(3)	Sodium chlorate $NaClO_3$
$m\bar{3} = T_h$	0	3(1)	0	12(3)	Pyrite FeS_2
$432 = O$	0	3(1)	0	12(3)	Manganese β -Mn
$\bar{4}3m = T_d$	0	3(1)	3(1)	12(3)	Zincblende ZnS
$m\bar{3}m = O_h$	0	3(1)	0	12(3)	Rocksalt $NaCl$

