Second order nonlinear processes in optical crystals

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Part I. (6.12.2000)

the effective nonlinearity: symmetries, crystal classes and conventions

Part II. (13.12.2000)

- the phase-matching (collinear, non-collinear and quasi-phase matching)

- the bandwidths (acceptances): spectral, angular, temperature

- frequency conversion with ultrashort pulses

Literature:

1. R. W. Boyd, Nonlinear Optics, 1992
2. W. Kleber, Einführung in die Kristallographie, 1985
3. V. G. Dmitriev, G. G. Gurzadyan, D. N. Nikogosyan, Handbook of nonlinear optical crystals, 1999
4. R. L. Sutherland, Handbook of nonlinear optics, 1996

Linear optics:

$\vec{P} = \varepsilon_0 \chi^{(1)} \vec{E}$ with ε_0 : dielectric constant,

$\chi^{(1)}$ linear susceptibility

Nonlinear optics: (spatial dispersion neglected)

$$\begin{aligned}
\vec{P}(t) &= \vec{P}_L(t) + \vec{P}_{NL}(t) \\
&= \varepsilon_0 \int_{-\infty}^{t} \chi^{(1)}(t;t_1)\vec{E}(t_1)dt_1 + \varepsilon_0 \int\int_{-\infty}^{t} \chi^{(2)}(t;t_1,t_2)\vec{E}(t_1)\vec{E}(t_2)dt_1dt_2 \\
&\quad + \varepsilon_0 \int\int\int_{-\infty}^{t} \chi^{(3)}(t;t_1,t_2,t_3)\vec{E}(t_1)\vec{E}(t_2)\vec{E}(t_3)dt_1dt_2dt_3 \cdots
\end{aligned}$$

$\chi^{(2)}$ and $\chi^{(3)}$: 2-nd and 3-rd order nonlinear susceptibilities.

Assumption: non-resonant interaction, neglecting both losses and dispersion (instantaneous response).

This reduces the susceptibilities to constants:

$$\begin{aligned}
\vec{P} &= \vec{P}_L + \vec{P}_{NL} \\
&= \varepsilon_0(\chi^{(1)}\vec{E} + \chi^{(2)}\vec{E}\vec{E} + \chi^{(3)}\vec{E}\vec{E}\vec{E} + \cdots) \\
&= \sum_{n=1} \vec{P}^{(n)}
\end{aligned}$$

$\chi^{(2)}$-processes („three-photon-processes"): lowest order nonlinear effect in non-centrosymmetric media.

convention $\omega_1<\omega_2<\omega_3$ ($\lambda_1>\lambda_2>\lambda_3$).

SFG (sum-frequency generation) $\omega_3=\omega_2+\omega_1$

SHG (second harmonic generation) $\omega_3=2\omega_1 \equiv$ SFG ($\omega_1=\omega_2$).

DFG (difference-frequency generation): $\omega_1=\omega_3-\omega_2$ (or $\omega_2=\omega_3-\omega_1$)

OPG (optical parametric generation): only the pump wave at ω_3 is present and two new waves at ω_1 and ω_2 (idler and signal) are generated.

OPA (optical parametric amplification) $\equiv$ OPG + (weak) seed wave at ω_1 or ω_2.

DFG $\equiv$ OPA (???) Gain (DFG) $\approx$ 1 e.g. @ ω_2

Gain (OPA) >> 1 e.g. @ ω_2

OPO (optical parametric oscillator) $\equiv$ (OPG or OPA) + resonator

The wave equation (non-magnetic, non-conductive medium):

$$\mathrm{rot}\,\mathrm{rot}\,\vec{E} + \frac{1}{c^2}\frac{\partial^2\vec{E}}{\partial t^2} = -\frac{1}{\varepsilon_0 c^2}\frac{\partial^2\vec{P}}{\partial t^2}$$

leads with the ansatz for the polarization to:

$$\Delta\vec{E} - \frac{1}{c^2}\frac{\partial^2\vec{E}}{\partial t^2} - \frac{1}{\varepsilon_0 c^2}\frac{\partial^2\vec{P}_L}{\partial t^2} = \frac{1}{\varepsilon_0 c^2}\frac{\partial^2\vec{P}_{NL}}{\partial t^2}$$

$\vec{E}$ is real and a superposition of quasi-monochromatic and quasi-plane waves:

$$\vec{E}(\vec{r},t) = \sum_n \vec{E}_n(\vec{r},t) = \sum_n \vec{A}_n(\vec{r},t)\exp[i(\vec{k}_n\vec{r} - \omega_n t)] + \mathrm{c.c.}$$
$$= \sum_n \vec{E}(\omega_n)e^{-i\omega_n t} + \mathrm{c.c} = \sum_n \vec{A}(\omega_n)e^{i(\vec{k}_n\vec{r}-\omega_n t)} + \mathrm{c.c.}$$

$\vec{A}_n(\vec{r},t) \equiv \vec{A}(\omega_n)$: slowly varying amplitudes

$\vec{k}_n$ [with $k_n = \omega_n n(\omega_n)/c$]: wave vectors at ω_n.

In $\vec{E}(\omega_n)$, $\vec{A}(\omega_n)$: *ω_n is a parameter and not an argument!!!*

$$\vec{P}(\vec{r},t) = \sum_n \vec{P}_n(\vec{r},t)\exp[i(\vec{k}_n\vec{r} - \omega_n t)] + \mathrm{c.c.}$$
$$= \sum_n \vec{P}(\omega_n)e^{-i\omega_n t} + \mathrm{c.c.}$$

Definition of $\chi^{(2)}_{ijk}(\omega_n + \omega_m, \omega_n, \omega_m)$:

$$P^{(2)}_i(\omega_n + \omega_m) = \varepsilon_0 \sum_{jk} \sum_{(mn)} \chi^{(2)}_{ijk}(\omega_n + \omega_m, \omega_n, \omega_m) E_j(\omega_n) E_k(\omega_m)$$

The summation (m,n) means, that $\omega_n + \omega_m$ remains constant though ω_n and ω_m are varied.

Other notations for $\chi^{(2)}(\omega_n + \omega_m, \omega_n, \omega_m)$:

$$\chi^{(2)}(-\omega_3; \omega_2, \omega_1) \qquad \text{or} \qquad \chi^{(2)}(\omega_3 = \omega_1 + \omega_2)$$

For SFG (ω_3=ω_1+ω_2) using the intrinsic permutation symmetry to sum over (m,n) we get:

$$P^{(2)}_i(\omega_3) = \varepsilon_0 D \sum_{jk} \chi^{(2)}_{ijk}(-\omega_3; \omega_1, \omega_2) E_j(\omega_1) E_k(\omega_2)$$

with $D = 1$ for $\omega_1 = \omega_2$

$= 2$ for $\omega_1 \neq \omega_2$

Intrinsic permutation symmetry: $\chi^{(2)}_{ijk}(\omega_n + \omega_m, \omega_n, \omega_m)$ remains unchanged exchanging the index pairs j,n and k,m.

Symmetries and number of independent components of $\chi^{(2)}$

$\chi^{(2)}$ consists of 12 tensors (differing in the permutation of the parameters ω_1, ω_2, ω_3) each of them having 27 (complex) cartesian components or we have:

648 real numbers

The reality of the fields:	**reduction factor of 2**
Intrinsic permutation symmetry:	**reduction factor of 2**
The neglect of losses leads to real $\chi^{(2)}$:	**reduction factor of 2**
and overall permutation symmetry:	**reduction factor of 3**

All frequencies far from optical resonances:

leads to frequency independent $\chi^{(2)}$-components („Kleinman-symmetry").

This means that the cartesian indices ijk can be exchanged without corresponding permutation of the frequency indices.

If $\chi^{(2)}$ are frequency independent and real we have **27** components (real numbers) which are reduced to **18** by the intrinsic symmetry. This justifies the introduction of the contracted d_{il}-tensor instead of $\chi^{(2)}_{ijk}$.

defining the nonlinear coefficients d_{ijk} as:

$$d_{ijk} = \frac{1}{2}\chi^{(2)}_{ijk}$$

We substitute d_{ijk} by d_{il} where

jk:	**11**	**22**	**33**	**23,32**	**31,13**	**12,21**
l:	**1**	**2**	**3**	**4**	**5**	**6**

These **18** components are reduced by the Kleinman symmetry to only **10**. e.g. $d_{24}=d_{223}=d_{322}=d_{32}$.

Miller's Rule:

$$d_{ijk}(\omega_1,\omega_2,\omega_3) = \Delta_{ijk}\chi^{(1)}(\omega_1)\chi^{(1)}(\omega_2)\chi^{(1)}(\omega_3)$$

with $\chi^{(1)}(\omega_n) = n^2(\omega_n) - 1$

where Δ_{ijk} is almost constant for all crystals without inversion centre: ($\approx$ 0.3 pm/V ±0.1pm/V).

Simplifications:

Collinear propagation in the z-direction ($\vec{k}_n\vec{r} \equiv k_n z$), field changes in the x- and y-directions neglected.

Slowly varying amplitude (SVA) approximation for the electric field:

$$\left|\frac{\partial^2}{\partial z^2}\vec{A}_n(z,t)\right| << \left|k_n \frac{\partial}{\partial z}\vec{A}_n(z,t)\right|, \left|\frac{\partial^2}{\partial t^2}\vec{A}_n(z,t)\right| << \left|\omega_n \frac{\partial}{\partial t}\vec{A}_n(z,t)\right|$$

and similar relations for the polarisation.

Birefringence neglected and scalar approximation implemented i.e. $A_n(z,t)$ denote further the x or y components of the linearly polarized fields $\vec{A}_n(z,t)$. *xyz is the laboratory system here*!

Reduction to a coupled system of 1-st order equations:

$$\left(\frac{\partial}{\partial z}+\frac{n_1}{c}\frac{\partial}{\partial t}\right)A_1(z,t) = i\frac{2\omega_1 d_{eff}}{n_1 c}A_3(z,t)A_2^*(z,t)\,e^{-i\Delta kz}$$

$$\left(\frac{\partial}{\partial z}+\frac{n_2}{c}\frac{\partial}{\partial t}\right)A_2(z,t) = i\frac{2\omega_2 d_{eff}}{n_2 c}A_3(z,t)A_1^*(z,t)\,e^{-i\Delta kz}$$

$$\left(\frac{\partial}{\partial z}+\frac{n_3}{c}\frac{\partial}{\partial t}\right)A_3(z,t) = i\frac{2\omega_3 d_{eff}}{n_3 c}A_1(z,t)A_2(z,t)\,e^{i\Delta kz}$$

c/n_n : phase velocities, $n_n=n(\omega_n)$: refractive indices

d_{eff} is a scalar which is a result of the summation over jk (in d_{ijk}) or over l (in d_{il}).

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Die 32 Kristallklassen (Punktgruppen)

Kristall-system	Nr.	Bezeichnung	Symbol inter-national	Symbol Schoen-flies	Allgemeine Form n[1])	Bild	Symmetrieelemente[2])	Zentrum	Enantio-morphie	Optische Aktivität	Piezo-elektri-zität	Pyro-elektri-zität
Triklin	1	triklin-pedial	1	C_1	1			−	+	+	+	+
	2	triklin-pinakoidal	$\bar{1}$	C_i	2	1.44	o	+	−	−	−	−
Monoklin	3	monoklin-sphenoidisch	2	C_2	2	1.40	⬮$_p$	−	+	+	+	+
	4	monoklin-domatisch	m	C_s	2	1.43	m	−	−	+	+	+
	5	monoklin-prismatisch	$2/m$	C_{2h}	4	1.52	⬮ + m	+	−	−	−	−
Rhombisch	6	rhombisch-disphenoidisch	222	D_2	4	1.63	⬮ + ⬮ + ⬮	−	+	+	+	−
	7	rhombisch-pyramidal	$mm2$	C_{2v}	4	(1.68a)	⬮$_p$ + m + m	−	−	+	+	+
	8	rhombisch-dipyramidal	mmm	D_{2h}	8	1.65	(⬮ + m) + (⬮ + m) + (⬮ + m)	+	−	−	−	−
Trigonal	9	trigonal-pyramidal	3	C_3	3	1.41	▲$_p$	−	+	+	+	+
	10	rhomboedrisch	$\bar{3}$	C_{3i}	6	1.46	△(≡ ▲ + o)	+	−	−	−	−
	11	trigonal-trapezoedrisch	32	D_3	6	1.77	▲ + 3 ⬮$_p$	−	+	+	+	−
	12	ditrigonal-pyramidal	$3m$	C_{3v}	6	(1.68d)	▲$_p$ + 3m	−	−	−	+	+
	13	ditrigonal-skalenoedrisch	$\bar{3}m$	D_{3d}	12	1.73	△(≡ ▲ + o) + 3(⬮ + m)	+	−	−	−	−
Hexagonal	14	hexagonal-pyramidal	6	C_6	6	1.41	⬢$_p$	−	+	+	+	+
	15	trigonal-dipyramidal	$\bar{6}$	C_{3h}	6	1.48	⬢(≡ ▲ + m)	−	−	−	+	−
	16	hexagonal-dipyramidal	$6/m$	C_{6h}	12	1.80	⬢ + m	+	−	−	−	−
	17	hexagonal-trapezoedrisch	622	D_6	12	1.85	⬢ + 3 ⬮ + 3 ⬮	−	+	+	+	−
	18	dihexagonal-pyramidal	$6mm$	C_{6v}	12	(1.68h)	⬢$_p$ + 3m + 3m	−	−	−	+	+
	19	ditrigonal-dipyramidal	$\bar{6}m2$	D_{3h}	12	1.83	⬢(≡ ▲ + m) + 3 ⬮$_p$ + 3m	−	−	−	+	−
	20	dihexagonal-dipyramidal	$6/mmm$	D_{6h}	24	1.86	(⬢ + m) + 3(⬮ + m) + 3(⬮ + m)	+	−	−	−	−
Tetragonal	21	tetragonal-pyramidal	4	C_4	4	1.41	◆$_p$	−	+	+	+	+
	22	tetragonal-disphenoidisch	$\bar{4}$	S_4	4	1.47	◈	−	−	+	+	−
	23	tetragonal-dipyramidal	$4m$	C_{4h}	8	1.91	◆ + m	+	−	−	−	−
	24	tetragonal-trapezoedrisch	422	D_4	8	1.96	◆ + 2 ⬮ + 2 ⬮	−	+	+	+	−
	25	ditetragonal-pyramidal	$4mm$	C_{4v}	8	(1.68f)	◆$_p$ + 2m + 2m	−	−	−	+	+
	26	tetragonal-skalenoedrisch	$\bar{4}2m$	D_{2d}	8	1.94	◈ + 2 ⬮ + 2m	−	−	+	+	−
	27	ditetragonal-dipyramidal	$4/mmm$	D_{4h}	16	1.98	(◆ + m) + 2(⬮ + m) + 2(⬮ + m)	+	−	−	−	−
Kubisch	28	tetraedrisch-pentagondodekaedrisch	23	T	12	1.102	3 ⬮ + 4 ▲$_p$	−	+	+	+	−
	29	disdodekaedrisch	$m\bar{3}$	T_h	24	1.105	3(⬮ + m) + 4 △	+	−	−	−	−
	30	pentagon-ikositetraedrisch	432	O	24	1.109	3 ◆ + 4 ▲ + 6 ⬮	−	+	+	−	−
	31	hexakistetraedrisch	$\bar{4}3m$	T_d	24	1.107	3 ◈ + 4 ▲$_p$ + 6m	−	−	−	+	−
	32	hexakisoktaedrisch	$m\bar{3}m$	O_h	48	1.110	3(◆ + m) + 4 △ + 6(⬮ + m)	+	−	−	−	−
								11	11	15	20	10

biaxial

uniaxial

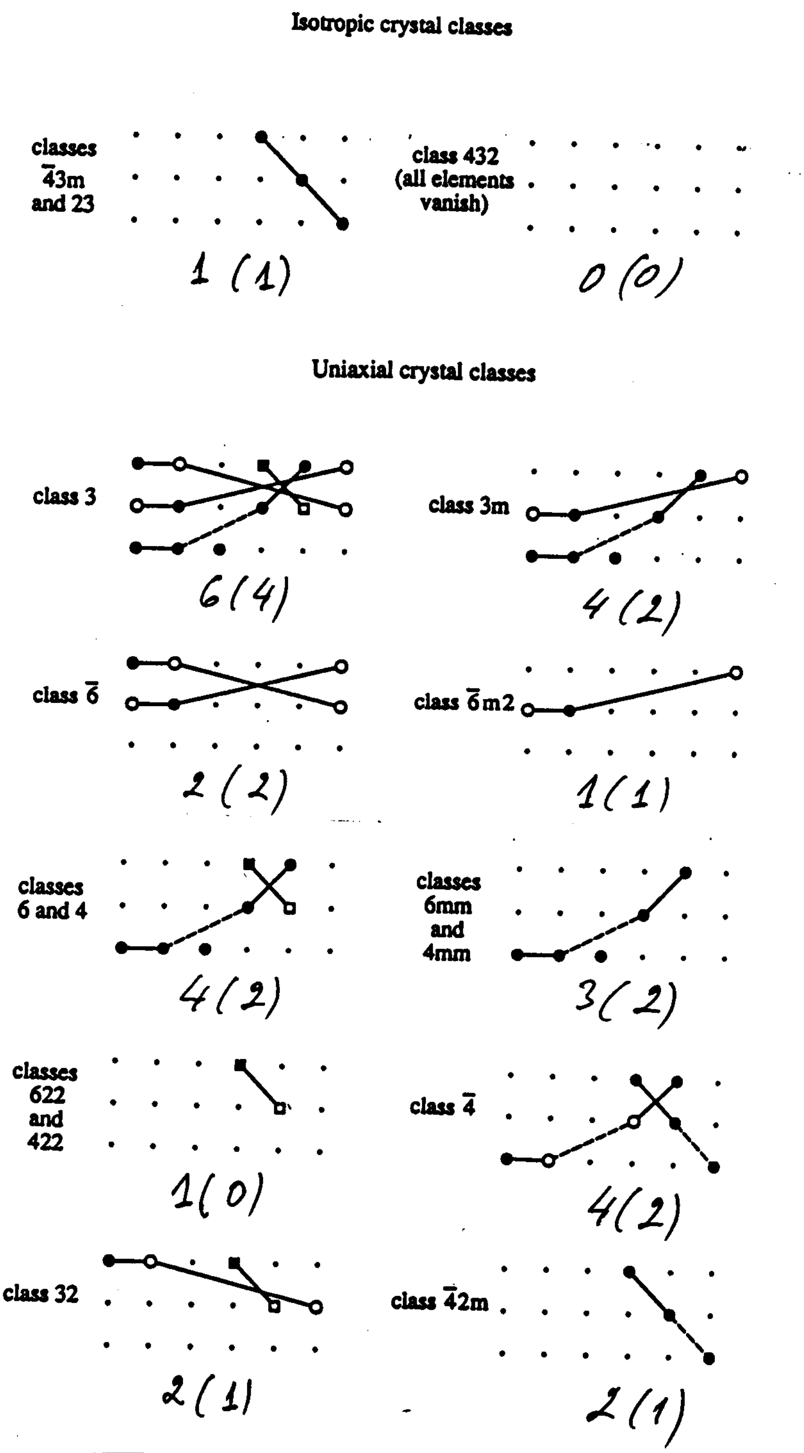
isotropic

V

[1]) n = Zähligkeit (Flächenzahl) der allgemeinen Form

[2]) Erläuterung der Symbole im Bild 1.51; p polare Achse

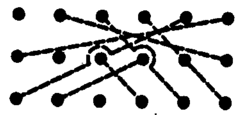
21



Form of the d_{il} matrix for the 21 crystal classes that lack inversion symmetry. Small dot: zero coefficient; large symbol: nonzero coefficient; square: coefficient that is zero when Kleinman's symmetry condition is valid; connected symbols: numerically equal coefficients, but the open-symbol coefficient is opposite in sign to the closed symbol to which it is joined. Dashed connections are valid only under Kleinman's symmetry conditions.

Biáxial crystal classes

class 1

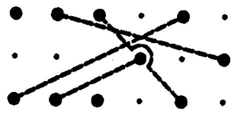


18 (12)

class 2

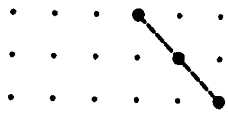
8 (5)

class m



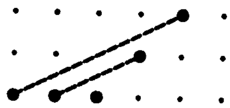
10 (6)

class 222



3 (1)

class mm2



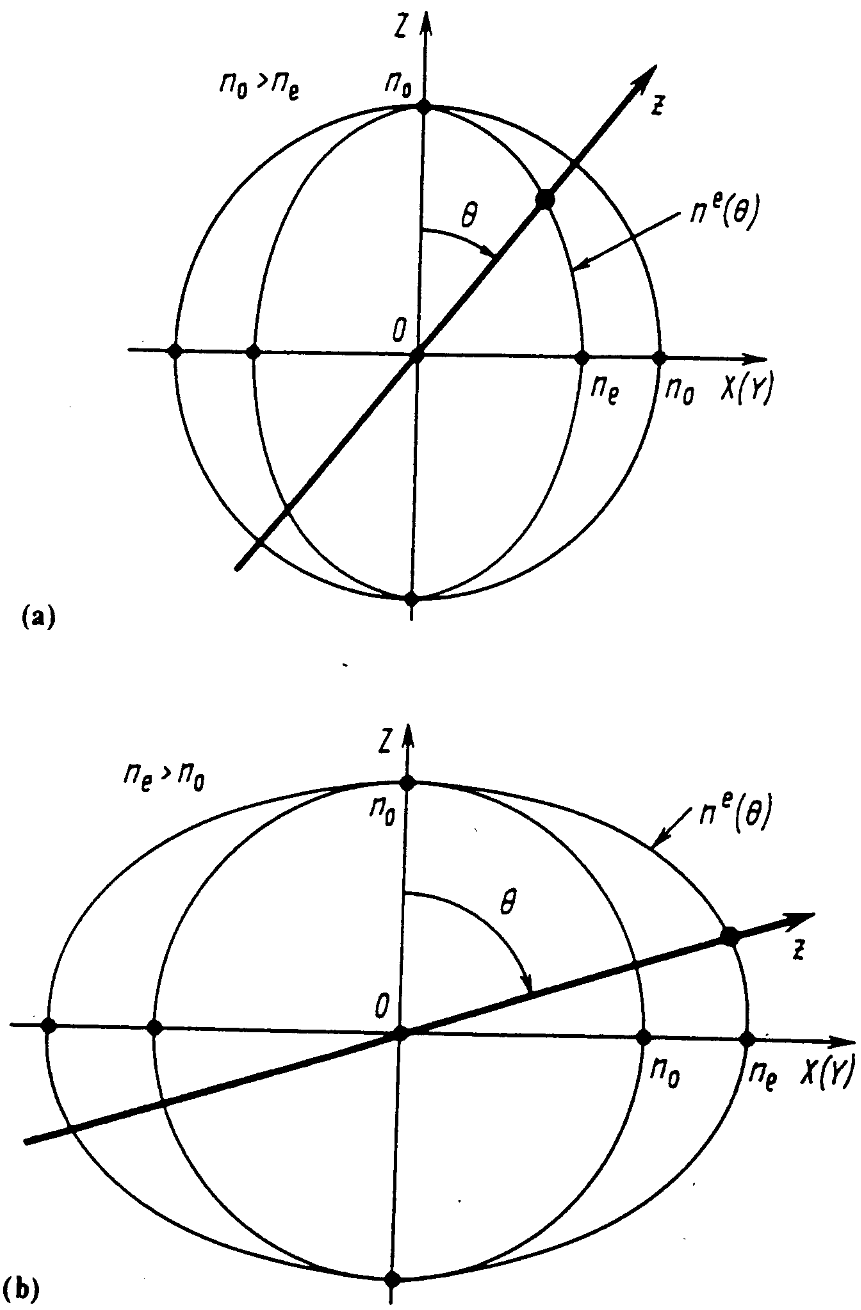
5 (3)

below: number of independent tensor components

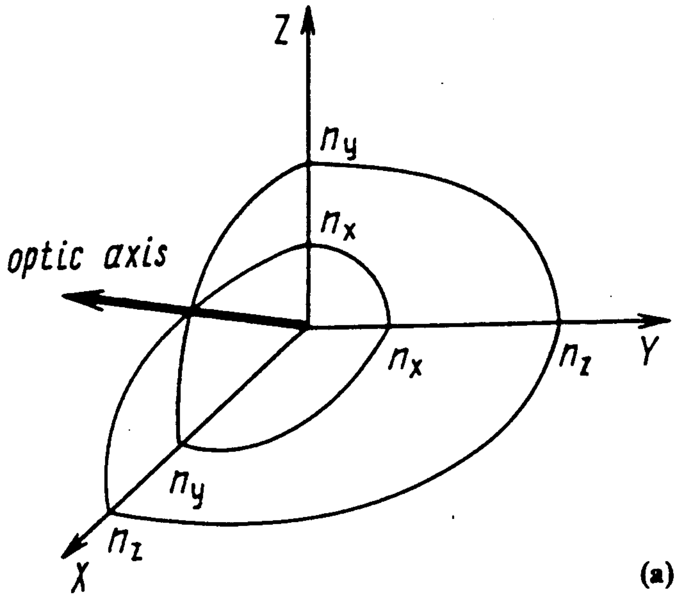
in brackets (+ Kleinman symmetry)

Conventions (just the most widely spread):

1. a,b,c denote the crystallographic axes
   (not necessarily orthonormalized frame)
2. X,Y,Z (or traditionally x,y,z) denote the crystallo-optical, dielectric, or principal optic axes frame (orthonormalized) where the linear susceptibility is diagonalized and where the polar angles are θ and ϕ are defined.
3. The right-hand frame X,Y,Z (x,y,z) is defined in biaxial crystals by either $n_X<n_Y<n_Z$ or $n_X>n_Y>n_Z$ (one of them arbitrarily chosen) where the principal refractive index values are for polarization parallel to the corresponding axis.
   This guarantees that the two optical axes lie in the XZ plane and $V_Z \equiv \Omega$ is the angle with the Z axis.
4. In uniaxial crystals Z denotes the optical axis ($\equiv$ with the crystallographic axis of highest symmetry) and we have:
   $n_X=n_Y=n_o$, $n_Z=n_e$
5. Negative (positive) uniaxial crystals are defined by
   $n_o>n_e$ ($n_e>n_o$)
   Negative (positive) biaxial crystals are defined by the bisectrix of the acute angle between the optical axes: if it concides with n_{min} (n_{max}) the crystal is negative (positive).

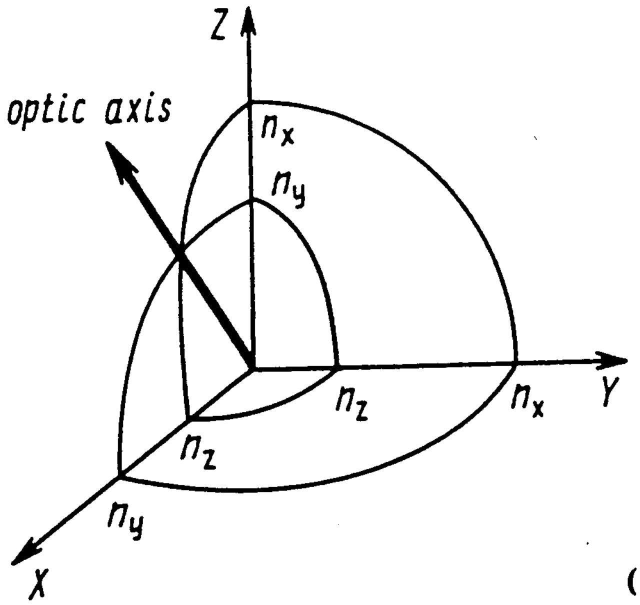


Dependence of refractive index on light propagation direction and polarization (index surface) in negative (a) and positive (b) uniaxial crystals



(a)

$$\sin V_Z = \frac{n_Z(n_Y^2 - n_X^2)^{1/2}}{n_Y(n_Z^2 - n_X^2)^{1/2}}$$



(b)

$$\cos V_Z = \frac{n_X(n_Y^2 - n_Z^2)^{1/2}}{n_Y(n_X^2 - n_Z^2)^{1/2}}$$

Dependence of refractive index on light propagation direction and polarization (index surface) in biaxial crystals under the following relations between principal values of refractive indices: **a)** $n_X < n_Y < n_Z$; **b)** $n_X > n_Y > n_Z$.

Formulas for d_{eff} in Uniaxial Crystals for the Different Types of Angle Phase Matching

Crystal class	Type I (ooe)	Type II (oeo or eoo)
4, 6	$d_{31} \sin\theta$	$d_{15} \sin\theta$
422, 622	0	0
$4mm$, $6mm$	$d_{31} \sin\theta$	$d_{15} \sin\theta$
$\bar{6}m2$	$-d_{22} \cos\theta \sin 3\phi$	$-d_{22} \cos\theta \sin 3\phi$
$3m$	$d_{31} \sin\theta - d_{22} \cos\theta \sin 3\phi$	$d_{15} \sin\theta - d_{22} \cos\theta \sin 3\phi$
$\bar{6}$	$(d_{11} \cos 3\phi - d_{22} \sin 3\phi) \cos\theta$	$(d_{11} \cos 3\phi - d_{22} \sin 3\phi) \cos\theta$
3	$(d_{11} \cos 3\phi - d_{22} \sin 3\phi) \cos\theta + d_{31} \sin\theta$	$(d_{11} \cos 3\phi - d_{22} \sin 3\phi) \cos\theta + d_{15} \sin\theta$
32	$d_{11} \cos\theta \cos 3\phi$	$d_{11} \cos\theta \cos 3\phi$
$\bar{4}$	$-(d_{31} \cos 2\phi + d_{36} \sin 2\phi) \sin\theta$	$-(d_{14} \sin 2\phi + d_{15} \cos 2\phi) \sin\theta$
$\bar{4}2m$	$-d_{36} \sin\theta \sin 2\phi$	$-d_{14} \sin\theta \sin 2\phi$
	Type I (eeo)	Type II (eoe or oee)
4, 6	$-d_{14} \sin 2\theta$	$d_{14} \sin\theta \cos\theta$
422, 622	$-d_{14} \sin 2\theta$	$d_{14} \sin\theta \cos\theta$
$4mm$, $6mm$	0	0
$\bar{6}m2$	$d_{22} \cos^2\theta \cos 3\phi$	$d_{22} \cos^2\theta \cos 3\phi$
$3m$	$d_{22} \cos^2\theta \cos 3\phi$	$d_{22} \cos^2\theta \cos 3\phi$
$\bar{6}$	$(d_{11} \sin 3\phi + d_{22} \cos 3\phi) \cos^2\theta$	$(d_{11} \sin 3\phi + d_{22} \cos 3\phi) \cos^2\theta$
3	$(d_{11} \sin 3\phi + d_{22} \cos 3\phi) \cos^2\theta - d_{14} \sin 2\theta$	$(d_{11} \sin 3\phi + d_{22} \cos 3\phi) \cos^2\theta + d_{14} \sin\theta \cos\theta$
32	$d_{11} \cos^2\theta \sin 3\phi - d_{14} \sin 2\theta$	$d_{11} \cos^2\theta \sin 3\phi + \frac{1}{2} d_{14} \sin 2\theta$
$\bar{4}$	$(d_{14} \cos 2\phi - d_{15} \sin 2\phi) \sin 2\theta$	$\frac{1}{2}[(d_{14} + d_{36}) \cos 2\phi - (d_{15} + d_{31}) \sin 2\phi] \sin 2\theta$
$\bar{4}2m$	$d_{14} \sin 2\theta \cos 2\phi$	$\frac{1}{2}(d_{14} + d_{36}) \sin 2\theta \cos 2\phi$

Formulas for d_{eff} in Uniaxial Crystals for the Different Types of Angle Phase Matching when Kleinman Symmetry Holds

Crystal class	ooe, oeo, eoo	eeo, eoe, oee
4, 6	$d_{15} \sin\theta$	0
422, 622	0	0
$4mm$, $6mm$	$d_{15} \sin\theta$	0
$\bar{6}m2$	$-d_{22} \cos\theta \sin 3\phi$	$d_{22} \cos^2\theta \cos 3\phi$
$3m$	$d_{15} \sin\theta - d_{22} \cos\theta \sin 3\phi$	$d_{22} \cos^2\theta \cos 3\phi$
$\bar{6}$	$(d_{11} \cos 3\phi - d_{22} \sin 3\phi) \cos\theta$	$(d_{11} \sin 3\phi + d_{22} \cos 3\phi) \cos^2\theta$
3	$(d_{11} \cos 3\phi - d_{22} \sin 3\phi) \cos\theta + d_{31} \sin\theta$	$(d_{11} \sin 3\phi + d_{22} \cos 3\phi) \cos^2\theta$
32	$d_{11} \cos\theta \cos 3\phi$	$d_{11} \cos^2\theta \sin 3\phi$
$\bar{4}$	$-(d_{14} \sin 2\phi + d_{15} \cos 2\phi) \sin\theta$	$(d_{14} \cos 2\phi - d_{15} \sin 2\phi) \sin 2\theta$
$\bar{4}2m$	$-d_{14} \sin\theta \sin 2\phi$	$d_{14} \sin 2\theta \cos 2\phi$

FORM OF THE SHG-TENSOR FOR THE VARIOUS CRYSTAL CLASSES

TRICLINIC SYSTEM

Class 1 – C_1

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

MONOCLINIC SYSTEM

Class m – C_s

$$\begin{bmatrix} d_{11} & d_{12} & d_{13} & 0 & 0 & d_{16} \\ d_{21} & d_{22} & d_{23} & 0 & 0 & d_{26} \\ 0 & 0 & 0 & d_{34} & d_{35} & 0 \end{bmatrix} \quad m \perp Z$$

Class m – C_s

$$\begin{bmatrix} d_{11} & d_{12} & d_{13} & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{24} & 0 & d_{26} \\ d_{31} & d_{32} & d_{33} & 0 & d_{35} & 0 \end{bmatrix} \quad m \perp Y$$

Class 2 – C_2

$$\begin{bmatrix} 0 & 0 & 0 & d_{14} & d_{15} & 0 \\ 0 & 0 & 0 & d_{24} & d_{25} & 0 \\ d_{31} & d_{32} & d_{33} & 0 & 0 & d_{36} \end{bmatrix} \quad 2 \parallel Z$$

Class 2 – C_2

$$\begin{bmatrix} 0 & 0 & 0 & d_{14} & 0 & d_{16} \\ d_{21} & d_{22} & d_{23} & 0 & d_{25} & 0 \\ 0 & 0 & 0 & d_{34} & 0 & d_{36} \end{bmatrix} \quad 2 \parallel Y$$

(IRE-convention)

ORTHORHOMBIC SYSTEM

Class $mm2$ – C_{2v}

$$\begin{bmatrix} 0 & 0 & 0 & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{24} & 0 & 0 \\ d_{31} & d_{32} & d_{33} & 0 & 0 & 0 \end{bmatrix}$$

Class 222 – D_2

$$\begin{bmatrix} 0 & 0 & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{25} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{36} \end{bmatrix}$$

TETRAGONAL SYSTEM

Class 4 – C_4

$$\begin{bmatrix} 0 & 0 & 0 & d_{14} & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & -d_{14} & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{bmatrix}$$

Class $\bar{4}$ – S_4

$$\begin{bmatrix} 0 & 0 & 0 & d_{14} & d_{15} & 0 \\ 0 & 0 & 0 & -d_{15} & d_{14} & 0 \\ d_{31} & -d_{31} & 0 & 0 & 0 & d_{36} \end{bmatrix}$$

Class $4mm$ – C_{4v}

$$\begin{bmatrix} 0 & 0 & 0 & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{36} \end{bmatrix}$$

Class $\bar{4}2m$ – D_{2d}

$$\begin{bmatrix} 0 & 0 & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{36} \end{bmatrix}$$

Class 422 – D_4

$$\begin{bmatrix} 0 & 0 & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

TRIGONAL SYSTEM

Class 3 – C_3

$$\begin{bmatrix} d_{11} & -d_{11} & 0 & d_{14} & d_{15} & -d_{22} \\ -d_{22} & d_{22} & 0 & d_{15} & -d_{14} & -d_{11} \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{bmatrix}$$

Class $3m$ – C_{3v}

$$\begin{bmatrix} 0 & 0 & 0 & 0 & d_{15} & -d_{22} \\ -d_{22} & d_{22} & 0 & d_{15} & 0 & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{bmatrix} \quad m \perp X$$

(IRE-convention)

FORM OF THE SHG-TENSOR FOR THE VARIOUS CRYSTAL CLASSES

Class $3m$ – C_{3v}

$$\begin{bmatrix} d_{11} & -d_{11} & 0 & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & 0 & -d_{11} \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{bmatrix} \quad m \perp Y$$

Class 32 – D_3

$$\begin{bmatrix} d_{11} & -d_{11} & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14} & -d_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

HEXAGONAL SYSTEM

Class $\bar{6}$ – C_{3h}

$$\begin{bmatrix} d_{11} & -d_{11} & 0 & 0 & 0 & -d_{22} \\ -d_{22} & d_{22} & 0 & 0 & 0 & -d_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Class 6 – C_6

$$\begin{bmatrix} 0 & 0 & 0 & d_{14} & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & -d_{14} & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{bmatrix}$$

Same as Class 4 – C_4

Class $\bar{6}m2$ – D_{3h}

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -d_{22} \\ -d_{22} & d_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad m \perp X$$

(IRE-convention)

Class $\bar{6}m2$ – D_{3h}

$$\begin{bmatrix} d_{11} & -d_{11} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -d_{11} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad m \perp Y$$

Class $6mm$ – C_{6v}

$$\begin{bmatrix} 0 & 0 & 0 & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & 0 & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{bmatrix}$$

Same as Class $4mm$ – D_{4v}

HEXAGONAL SYSTEM

Class 622 – D_6

$$\begin{bmatrix} 0 & 0 & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Same as Class 422 – D_4

CUBIC SYSTEM

Class 23 – T

$$\begin{bmatrix} 0 & 0 & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{14} \end{bmatrix}$$

Class $\bar{4}3m$ – T_d

$$\begin{bmatrix} 0 & 0 & 0 & d_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{14} \end{bmatrix}$$

Class 432 – O

All elements vanish

General case

Effective second-order nonlinear coefficients d_{eff} for biaxial crystals. under Kleinman symmetry

	Phase matching, type I	Phase matching, type II
222-orthorhombic	$d_{36}[\sin 2\theta \cos 2\phi \cos\delta (3\sin^2\delta - 1)$ $+ \sin\theta \sin 2\phi \sin\delta (3\cos^2\theta \cos^2\delta + 3\cos^2\delta - 1)]$	$d_{36}[\sin 2\theta \cos 2\phi \sin\delta (3\cos^2\delta - 1)$ $- \sin\theta \sin 2\phi \cos\delta (3\cos^2\theta \sin^2\delta + 3\sin^2\delta - 1)]$
$mm2$-orthorhombic	$(d_{32} - d_{31}) \cos\theta \sin\theta \sin 2\phi \cos\delta \sin^2\delta$ $+(d_{15} - d_{24}) \cos\theta \sin\theta \sin 2\phi \cos\delta \cos 2\delta$ $+(d_{32}\cos^2\phi + d_{31}\sin^2\phi) \sin\theta \sin^3\delta$ $+(d_{32}\sin^2\phi + d_{31}\cos^2\phi) \cos^2\theta \sin\theta \cos^2\delta \sin\delta$ $-2(d_{24}\cos^2\phi + d_{15}\sin^2\phi) \sin\theta \cos^2\delta \sin\delta$ $+2(d_{24}\sin^2\phi + d_{15}\cos^2\phi) \cos^2\theta \sin\theta \cos^2\delta \sin\delta$ $+d_{33}\sin^3\theta \cos^2\delta \sin\delta$	$(d_{32} - d_{31}) \cos\theta \sin\theta \cos\phi \sin\phi \sin\delta \cos 2\delta$ $+(d_{24} - d_{15}) \cos\theta \sin\theta \cos\phi \sin\phi \sin\delta (4\cos^2\delta - 1)$ $-(d_{31}\cos^2\phi + d_{32}\sin^2\phi) \cos^2\theta \sin\theta \cos\delta \sin^2\delta$ $+(d_{31}\sin^2\phi + d_{32}\cos^2\phi) \sin\theta \cos\delta \sin^2\delta$ $-2(d_{15}\cos^2\phi + d_{24}\sin^2\phi) \cos^2\theta \sin\theta \cos\delta \sin^2\delta$ $-(d_{15}\sin^2\phi + d_{24}\cos^2\phi) \sin\theta \cos\delta \cos 2\delta$ $-d_{33}\sin^3\theta \cos\delta \sin^2\delta$.
2-monoclinic	$-(d_{22}\sin^2\phi + 3d_{21}\cos^2\phi) \cos^3\theta \sin\phi \sin\delta \cos^2\delta$ $-[d_{22}\cos^2\phi + d_{21}(3\sin^2\phi - 2)] \cos\theta \sin\phi \sin^3\delta$ $+2[d_{22}\cos^2\phi - d_{21}(3\cos^2\phi - 1)] \cos\theta \sin\phi \sin\delta \cos^2\delta$ $-2[d_{22}\sin^2\phi - d_{21}(3\sin^2\phi - 1)] \cos^2\theta \cos\phi \sin^2\delta \cos\delta$ $-[d_{22}\sin^2\phi + d_{21}(\sin^2\phi + 1)] \cos^2\theta \cos\phi \cos^3\delta$ $-d_{34}\sin^2\theta \cos\delta [3\cos\theta \sin\phi \sin\delta \cos\delta - \cos\phi (3\cos^2\delta - 2)]$ $+d_{36}[\sin 2\theta \cos 2\phi \cos\delta (3\sin^2\delta - 1)$ $+\sin\theta \sin 2\phi \sin\delta (3\cos^2\theta \cos^2\delta + 3\cos^2\delta - 1)]$	$(d_{22}\sin^2\phi + 3d_{21}\cos^2\phi) \cos^3\theta \sin\phi \sin^2\delta \cos\delta$ $+[d_{22}\cos^2\phi + d_{21}(3\sin^2\phi - 2)] \cos\theta \sin\phi \cos^3\delta$ $-2[d_{22}\cos^2\phi - d_{21}(3\cos^2\phi - 1)] \cos\theta \sin\phi \sin^2\delta \cos\delta$ $-2[d_{22}\sin^2\phi - d_{21}(3\cos^2\phi - 1)] \cos^2\theta \cos\phi \sin\delta \cos^2\delta$ $-[d_{22}\sin^2\phi + d_{21}(\sin^2\phi + 1)] \cos^2\theta \cos\phi \sin^3\delta$ $+d_{34}\sin^2\theta \sin\delta [3\cos\theta \sin\phi \sin\delta \cos\delta + \cos\phi (3\sin^2\delta - 2)]$ $+d_{36}[\sin 2\theta \cos 2\phi \sin\delta (3\cos^2\delta - 1)$ $-\sin\theta \sin 2\phi \cos\delta (3\cos^2\theta \sin^2\delta + 3\sin^2\delta - 1)]$

Here: d_{il} defined in X, Y, Z

or $X, Y, Z = a, b, c$ for 222/mm2

$$\cot 2\delta = \frac{\cot^2\Omega \sin^2\theta - \cos^2\theta \cos^2\phi + \sin^2\phi}{\cos\theta - \sin 2\phi},$$

where Ω is the angle between the Z axis and the optic axis.

mm2

$d_{caa} = d_{31}$; $d_{cbb} = d_{32}$; $d_{ccc} = d_{33}$;
$d_{aac} = d_{15}$; $d_{bbc} = d_{24}$.

Kleinman:
$d_{15} = d_{31}$
$d_{24} = d_{32}$

in Principal Planes:

Components of d_{ijk} tensor in the dielectric coordinate system for different assignments between the dielectric and crystallographic reference frames

N	Assignment	$d_{caa} = d_{31}$	$d_{cbb} = d_{32}$	$d_{ccc} = d_{33}$	$d_{aac} = d_{15}$	$d_{bbc} = d_{24}$
1	$X,Y,Z \rightarrow a,b,c$	d_{ZXX}	d_{ZYY}	d_{ZZZ}	d_{XXZ}	d_{YYZ}
2	$X,Y,Z \rightarrow b,a,c$	d_{ZYY}	d_{ZXX}	d_{ZZZ}	d_{YYZ}	d_{XXZ}
3	$X,Y,Z \rightarrow a,c,b$	d_{YXX}	d_{YZZ}	d_{YYY}	d_{XXY}	d_{ZZY}
4	$X,Y,Z \rightarrow b,c,a$	d_{YZZ}	d_{YXX}	d_{YYY}	d_{ZZY}	d_{XXY}
5	$X,Y,Z \rightarrow c,b,a$	d_{XZZ}	d_{XYY}	d_{XXX}	d_{ZZX}	d_{YYX}
6	$X,Y,Z \rightarrow c,a,b$	d_{XYY}	d_{XZZ}	d_{XXX}	d_{YYX}	d_{ZZX}

The possible types of phase matching in the principal planes of the mm2 point group biaxial crystal for the case $n_X < n_Y < n_Z$

Assignment	Principal plane XY	YZ	XZ $\theta < V_Z$	XZ $\theta > V_Z$
$X,Y,Z \rightarrow a,b,c$	$\mathrm{II}^{(-)}$	$\mathrm{II}^{(+)}$	$\mathrm{I}^{(-)}$	$\mathrm{II}^{(+)}$
or $\rightarrow b,a,c$	oe-e,eo-e	oe-o, eo-o	oo-e	oe-o, eo-o
$X,Y,Z \rightarrow a,c,b$	$\mathrm{I}^{(-)}$	$\mathrm{II}^{(+)}$	$\mathrm{II}^{(-)}$	$\mathrm{I}^{(+)}$
or $\rightarrow b,c,a$	oo-e	oe-o,eo-o	oe-e,eo-e	ee-o
$X,Y,Z \rightarrow c,b,a$	$\mathrm{I}^{(-)}$	$\mathrm{I}^{(+)}$	$\mathrm{I}^{(-)}$	$\mathrm{II}^{(+)}$
or $\rightarrow c,a,b$	oo-e	ee-o	oo-e	oe-o,eo-o

The possible types of phase matching in the principal planes of the mm2 point group biaxial crystal for the case $n_X > n_Y > n_Z$

Assignment	Principal plane XY	YZ	XZ $\theta < V_Z$	XZ $\theta > V_Z$
$X,Y,Z \rightarrow a,b,c$	$\mathrm{I}^{(+)}$	$\mathrm{I}^{(-)}$	$\mathrm{II}^{(+)}$	$\mathrm{I}^{(-)}$
or $\rightarrow$ b,a,c	ee-o	oo-e	oe-o,eo-o	oo-e
$X,Y,Z \rightarrow a,c,b$	$\mathrm{II}^{(+)}$	$\mathrm{I}^{(-)}$	$\mathrm{I}^{(+)}$	$\mathrm{II}^{(-)}$
or $\rightarrow b,c,a$	oe-o,eo-o	oo-e	ee-o	oe-e,eo-e
$X,Y,Z \rightarrow c,b,a$	$\mathrm{II}^{(+)}$	$\mathrm{II}^{(-)}$	$\mathrm{II}^{(+)}$	$\mathrm{I}^{(-)}$
or $\rightarrow c,a,b$	oe-o,eo-o	oe-e,eo-e	oe-o,eo-o	oo-e

polarization: o: $\perp$ to plane, e: in plane

mm2-class, $V_Z \equiv \Omega$
Kleinman symmetry

The d_{eff} expressions for the principal planes of the mm2 point group biaxial crystal in the case $n_X < n_Y < n_Z$

Assignment	Plane	$d_{eff}^{ss\text{-}f}$ (Type I)	$d_{eff}^{sf\text{-}f}$ (Type II)
$X,Y,Z \to a,b,c$	XY	0	$d_{15}\sin^2\phi + d_{24}\cos^2\phi$
	YZ	0	$d_{15}\sin\theta$
	$XZ,\ \theta < V_Z$	$d_{32}\sin\theta$	0
	$XZ,\ \theta > V_Z$	0	$d_{24}\sin\theta$
$X,Y,Z \to b,a,c$	XY	0	$d_{24}\sin^2\phi + d_{15}\cos^2\phi$
	YZ	0	$d_{24}\sin\theta$
	$XZ,\ \theta < V_Z$	$d_{31}\sin\theta$	0
	$XZ,\ \theta > V_Z$	0	$d_{15}\sin\theta$
$X,Y,Z \to a,c,b$	XY	$d_{32}\cos\phi$	0
	YZ	0	$d_{15}\cos\theta$
	$XZ,\ \theta < V_Z$	0	$d_{24}\sin^2\theta + d_{15}\cos^2\theta$
	$XZ,\ \theta > V_Z$	$d_{32}\sin^2\theta + d_{31}\cos^2\theta$	0
$X,Y,Z \to b,c,a$	XY	$d_{31}\cos\phi$	0
	YZ	0	$d_{24}\cos\theta$
	$XZ,\ \theta < V_Z$	0	$d_{15}\sin^2\theta + d_{24}\cos^2\theta$
	$XZ,\ \theta > V_Z$	$d_{31}\sin^2\theta + d_{32}\cos^2\theta$	0
$X,Y,Z \to c,b,a$	XY	$d_{31}\sin\phi$	0
	YZ	$d_{31}\sin^2\theta + d_{32}\cos^2\theta$	0
	$XZ,\ \theta < V_Z$	$d_{32}\cos\theta$	0
	$XZ,\ \theta > V_Z$	0	$d_{24}\cos\theta$
$X,Y,Z \to c,a,b$	XY	$d_{32}\sin\phi$	0
	YZ	$d_{32}\sin^2\theta + d_{31}\cos^2\theta$	0
	$XZ,\ \theta < V_Z$	$d_{31}\cos\theta$	0
	$XZ,\ \theta > V_Z$	0	$d_{15}\cos\theta$

The d_{eff} expressions for the principal planes of the mm2 point group biaxial crystal in the case $n_X > n_Y > n_Z$

Assignment	Plane	$d_{eff}^{ss\text{-}f}$ (Type I)	$d_{eff}^{sf\text{-}f}$ (Type II)
$X,Y,Z \to a,b,c$	XY	$d_{31}\sin^2\phi + d_{32}\cos^2\phi$	0
	YZ	$d_{31}\sin\theta$	0
	$XZ,\ \theta < V_Z$	0	$d_{24}\sin\theta$
	$XZ,\ \theta > V_Z$	$d_{32}\sin\theta$	0
$X,Y,Z \to b,a,c$	XY	$d_{32}\sin^2\phi + d_{31}\cos^2\phi$	0
	YZ	$d_{32}\sin\theta$	0
	$XZ,\ \theta < V_Z$	0	$d_{15}\sin\theta$
	$XZ,\ \theta > V_Z$	$d_{31}\sin\theta$	0
$X,Y,Z \to a,c,b$	XY	0	$d_{24}\cos\phi$
	YZ	$d_{31}\cos\theta$	0
	$XZ,\ \theta < V_Z$	$d_{32}\sin^2\theta + d_{31}\cos^2\theta$	0
	$XZ,\theta > V_Z$	0	$d_{24}\sin^2\theta + d_{15}\cos^2\theta$
$X,Y,Z \to b,c,a$	XY	0	$d_{15}\cos\phi$
	YZ	$d_{32}\cos\theta$	0
	$XZ,\ \theta < V_Z$	$d_{31}\sin^2\theta + d_{32}\cos^2\theta$	0
	$XZ,\ \theta > V_Z$	0	$d_{15}\sin^2\theta + d_{24}\cos^2\theta$
$X,Y,Z \to c,b,a$	XY	0	$d_{15}\sin\phi$
	YZ	0	$d_{15}\sin^2\theta + d_{24}\cos^2\theta$
	$XZ,\ \theta < V_Z$	0	$d_{24}\cos\theta$
	$XZ,\ \theta > V_Z$	$d_{32}\cos\theta$	0
$X,Y,Z \to c,a,b$	XY	0	$d_{24}\sin\phi$
	YZ	0	$d_{24}\sin^2\theta + d_{15}\cos^2\theta$
	$XZ,\ \theta < V_Z$	0	$d_{15}\cos\theta$
	$XZ,\ \theta > V_Z$	$d_{31}\cos\theta$	0

222 d_{il} defined in a, b, c

for all asignments $X, Y, Z \to a, b, c$

Expressions for d_{eff} and possible types of phase matching in the principal planes of the 222 point group biaxial crystal when Kleinman symmetry relations are valid

Plane	$n_X < n_Y < n_Z$	$n_X > n_Y > n_Z$
XY	$d_{14} \sin 2\phi$, type $\mathrm{II}^{(-)}$	$-d_{14} \sin 2\phi$, type $\mathrm{I}^{(+)}$
YZ	$d_{14} \sin 2\theta$, type $\mathrm{I}^{(+)}$	$-d_{14} \sin 2\theta$, type $\mathrm{II}^{(-)}$
XZ, $\theta < V_Z$	$-d_{14} \sin 2\theta$, type $\mathrm{II}^{(-)}$	$d_{14} \sin 2\theta$, type $\mathrm{I}^{(+)}$
XZ, $\theta > V_Z$	$-d_{14} \sin 2\theta$, type $\mathrm{I}^{(+)}$	$d_{14} \sin 2\theta$, type $\mathrm{II}^{(-)}$

2 d_{il} defined directly in X, Y, Z

Expressions for d_{eff} and possible types of phase matching in the principal planes of the biaxial crystal of 2 point group when Klienman symmetry relations are valid and nonlinear coefficients are defined in dielectric reference frame

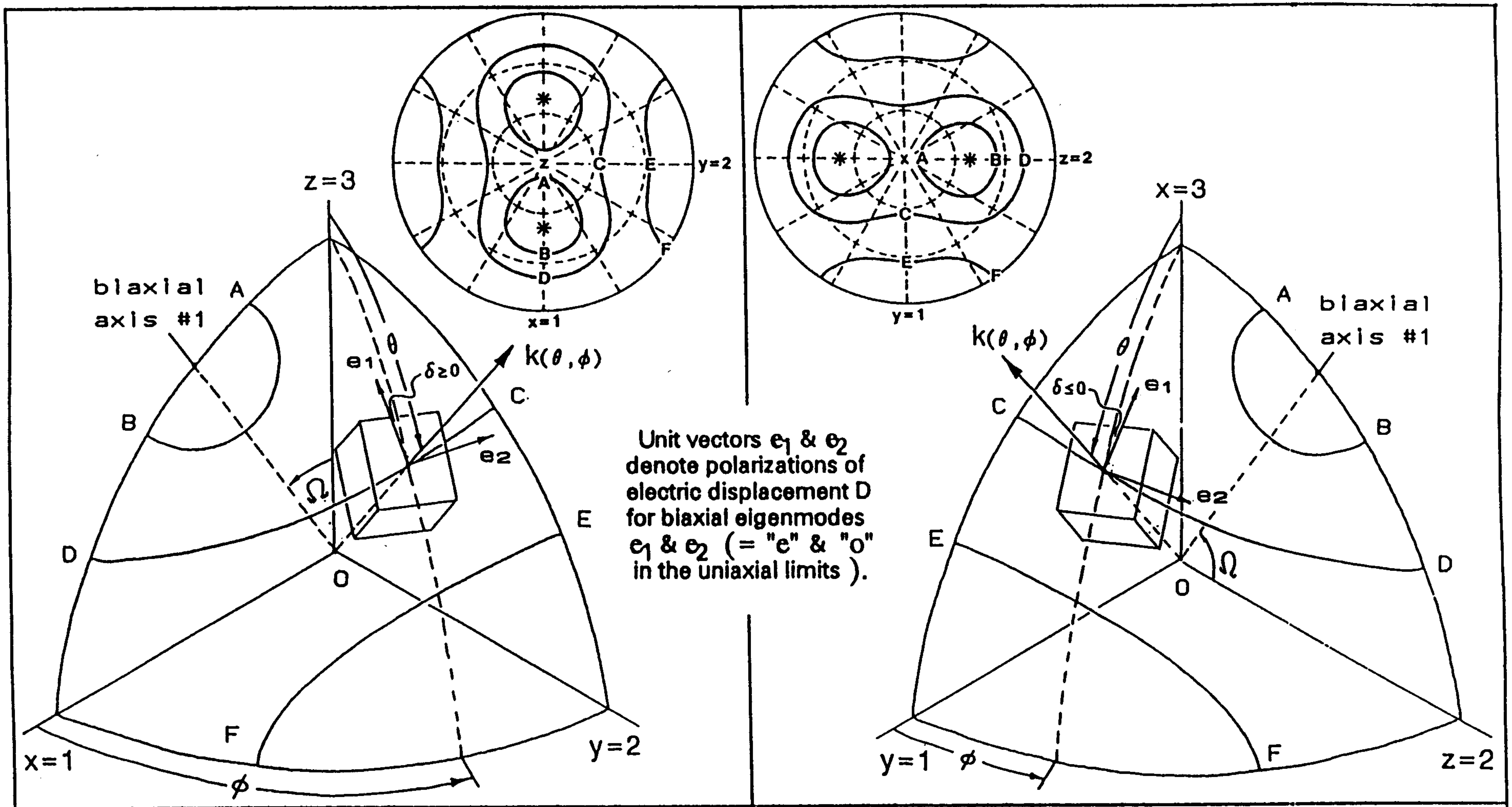
Plane	$n_X < n_Y < n_Z$	$n_X > n_Y > n_Z$
XY	$d_{25} \sin 2\phi$, type $\mathrm{II}^{(-)}$	$d_{25} \sin 2\phi$, type $\mathrm{I}^{(+)}$
	$d_{23} \cos \phi$, type $\mathrm{I}^{(-)}$	$d_{23} \cos \phi$, type $\mathrm{II}^{(+)}$
YZ	$d_{21} \cos \theta$, type $\mathrm{II}^{(+)}$	$d_{21} \cos \theta$, type $\mathrm{I}^{(-)}$
	$d_{25} \sin 2\theta$, type $\mathrm{I}^{(+)}$	$d_{25} \sin 2\theta$, type $\mathrm{II}^{(-)}$
XZ, $\theta < V_Z$	$d_{21} \cos^2 \theta + d_{23} \sin^2 \phi$	$d_{21} \cos^2 \theta + d_{23} \sin^2 \phi$
	$+d_{25} \sin 2\theta$, type $\mathrm{II}^{(-)}$	$+d_{25} \sin 2\theta$, type $\mathrm{I}^{(+)}$
XZ, $\theta > V_Z$	$d_{21} \cos^2 \theta + d_{23} \sin^2 \phi$	$d_{21} \cos^2 \theta + d_{23} \sin^2 \phi$
	$+d_{25} \sin 2\theta$, type $\mathrm{I}^{(+)}$	$+d_{25} \sin 2\theta$, type $\mathrm{II}^{(-)}$

It is our hope that IEEE/ANSI Std. 176-1987 (amended for orthorhombic class mm2) and other standards summarized below will be adopted by the nonlinear optics community:

1) $\lambda_1 \geq \lambda_2 > \lambda_3$ denote vacuum wavelengths for all interaction types: SHG, SFM, DFM, OPO, OPA.
2) *abc* denotes crystallographic axes (IEEE/ANSI).
3) $\alpha\beta\gamma$ denote interaxial angles (IEEE/ANSI).
4) *XYZ* denotes reporting frame for crystal tensor properties, such as nonlinear $d_{i\mu}$ (IEEE/ANSI).
5) *xyz* denotes principal optic axis frame (traditional).
6) $n_x \leq n_y \leq n_z$ denote refractive indexes for polarization along axes x, y, and z (traditional).
7) $123 = xyz/yzx =$ the POSITIVE/NEGATIVE NLO FRAME for θ, ϕ, δ, ρ reporting for POSITIVE/NEGATIVE crystals, where θ is measured from "3" toward the "12" plane and ϕ is measured from "1" toward "2", and where NLO crystal is considered POSITIVE/NEGATIVE according to $\Omega_{ave} \leq 45°$ or $\Omega_{ave} > 45°$ in a given interaction, but either NLO FRAME could be used in marginal cases.

Crystal System unit cell info	Class	*abc*-Identification				*XYZ*-Identification		
		c	a	b		X	Y	Z
Triclinic								
$c_O < a_O < b_O$	1						⟨010⟩	c
$\alpha, \beta > 90°$								
Monoclinic	2			2		⟨100⟩	b	c
$c_O < a_O$	m			⊥m		⟨100⟩	b	c
$\alpha, \gamma = 90°$								
$\beta > 90°$								
Orthorhombic	222	2	2	2		a	b	c
$c_O < a_O < b_O$	mm2	2				a	b	c
$\alpha, \beta, \gamma = 90°$	m2m			2		c	a	b
(see Note 1)	2mm		2			c	b	a
		c	a_1	a_2				
Tetragonal	4	4	†			a_1	a_2	c
$a_O = b_O$	$\bar{4}$	$\bar{4}$	†			a_1	a_2	c
$\alpha, \beta, \gamma = 90°$	422	4	2	2		a_1	a_2	c
	4mm	4	⊥m	⊥m		a_1	a_2	c
	$\bar{4}$2m	$\bar{4}$	2	2		†	†	c
		c	a_1	a_2	a_3			
Trigonal	3	3	†			a_1		c
†	32	3	2	2	2	a_1		c
	3m	3	⊥m	⊥m	⊥m	a_1		c
Hexagonal	6	6	†			a_1		c
†	$\bar{6}$	$\bar{6}$	†			a_1		c
$(a_O)_1 =$	622	6	2	2	2	a_1		c
$(a_O)_2 =$	6mm	6	⊥m	⊥m	⊥m	a_1		c
$(a_O)_3$	$\bar{6}$m2	$\bar{6}$	2	2	2	a_1	†	c
		a_1	a_2	a_3				
Cubic								
$a_O = b_O = c_O$	23	2	2	2		a_1	a_2	a_3
$\alpha, \beta, \gamma = 90°$	$\bar{4}$3m	$\bar{4}$	$\bar{4}$	$\bar{4}$		a_1	a_2	a_3

Note 1: Std. 176-1987 definitions of axes *abc* for the polar orthorhombic class (mm2/m2m/2mm) have not been embraced by the physics and engineering communities. Hence, we recommend that the NLO community and IEEE Standards Board adopt "$Z = c =$ polar (already a *de facto* standard), $X = a$, $Y = b$, $a_O < b_O$." This does not affect *XYZ*, and gives an automatic, convenient, mm2 designation to all crystals in this class.



POSITIVE NLO FRAME

Uniaxial Positive : $(n_x = n_y = n_o) < (n_z = n_e)$

Biaxial Positive : $n_x < n_y < n_z$, $\Omega_{ave} \leq 45°$

NEGATIVE NLO FRAME

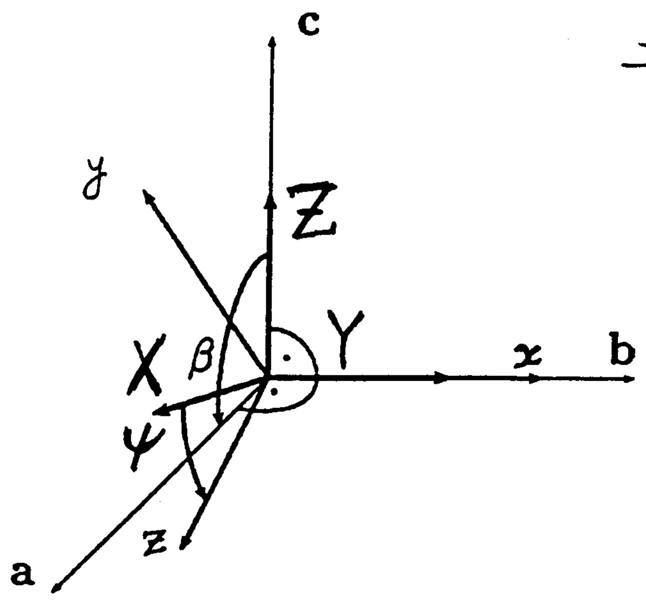
Uniaxial Negative : $(n_z = n_y = n_o) > (n_x = n_e)$

Biaxial Negative : $n_z > n_y > n_x$, $\Omega_{ave} > 45°$

(a) (b)

1st Octant (+ optional 4-octant stereonet) of proposed positive and negative NLO reporting frames.

BiB_3O_6 (2)



Orientation of the crystalophysical coordinate system XYZ assign-
ment of the main refractive indices x, y, z and definition of the dispersion angle ψ

1. xyz frame exhibits temperature and wavelength dispersion (the indicatrix rotates) with respect to the XYZ crystallophysical frame.

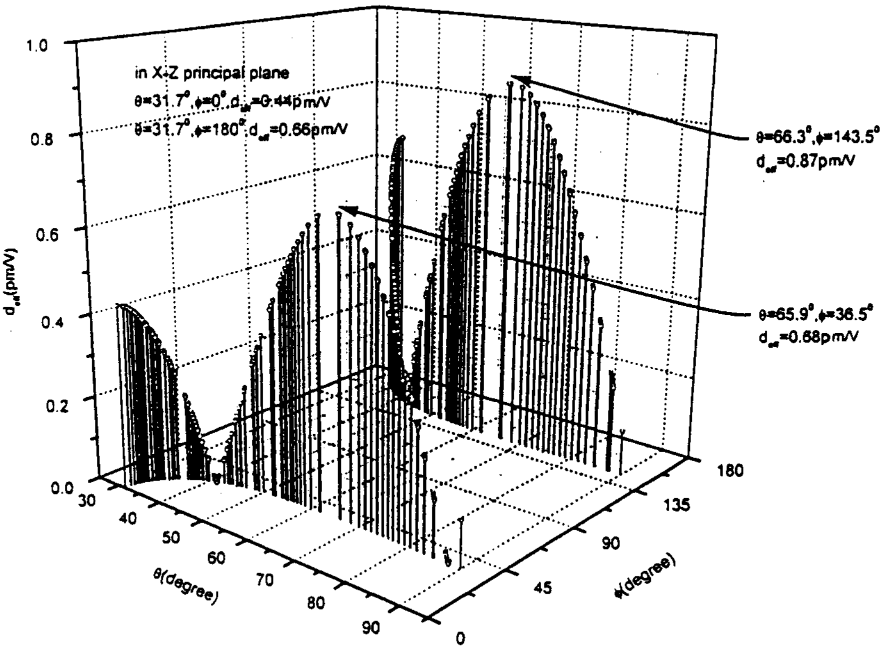
2. In the monoclinic classes 2 and m the rotation is arount the Y≡b axis which coincides with one principal optic (dielectric) axis and can be described by the additional angle $\psi(T,\lambda)$. There is an additional convention Z≡c.

3. In the triclinic class 1 we have only the second convention Z≡c, but none of the xyz axes coincides with any of the XYZ or abc axes. The rotation of the indicatrix xyz with respect to XYZ is generally described by two angles.

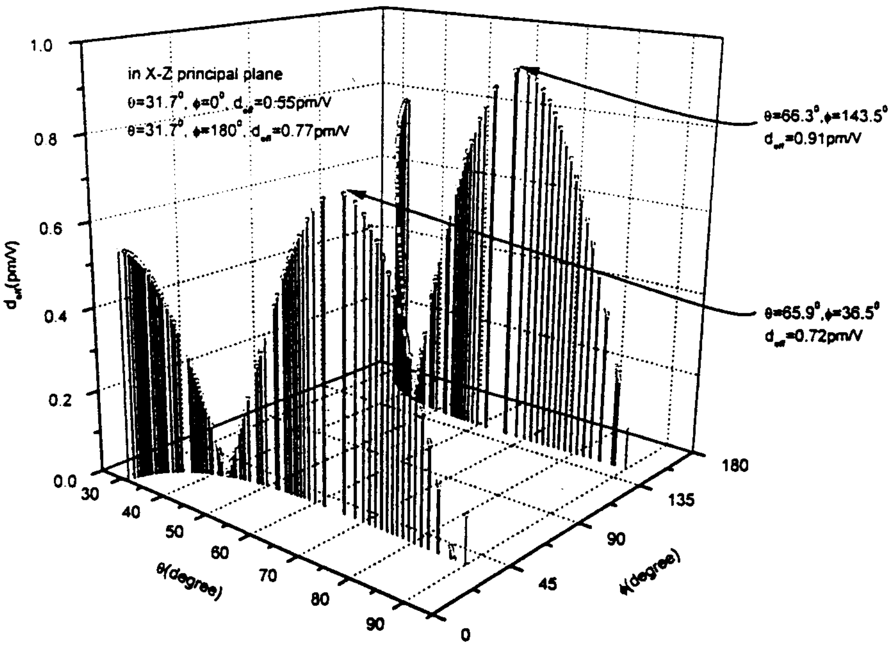
4. In the monoclinic and triclinic classes the maximum d_{eff} could be out of the principal planes and in general because of the low symmetry we have to consider more than one octants.

$YCa_4O(BO_3)_3 \equiv YCOB$ (m)

calculation of dil



(a)



(b)

(a) Three-dimensional space relationships between the d_{eff} coefficient and phase-matching angle (θ, φ) of YCOB with (a) d_{ij} coefficients calculated by the Gaussian 92 program and (b) d_{33} and d_{32} coefficients measured by the Maker fringes method and d_{12}, d_{11}, d_{13}, and d_{31} coefficients calculated by the Gaussian 92 program.

SHG @ 1064 nm