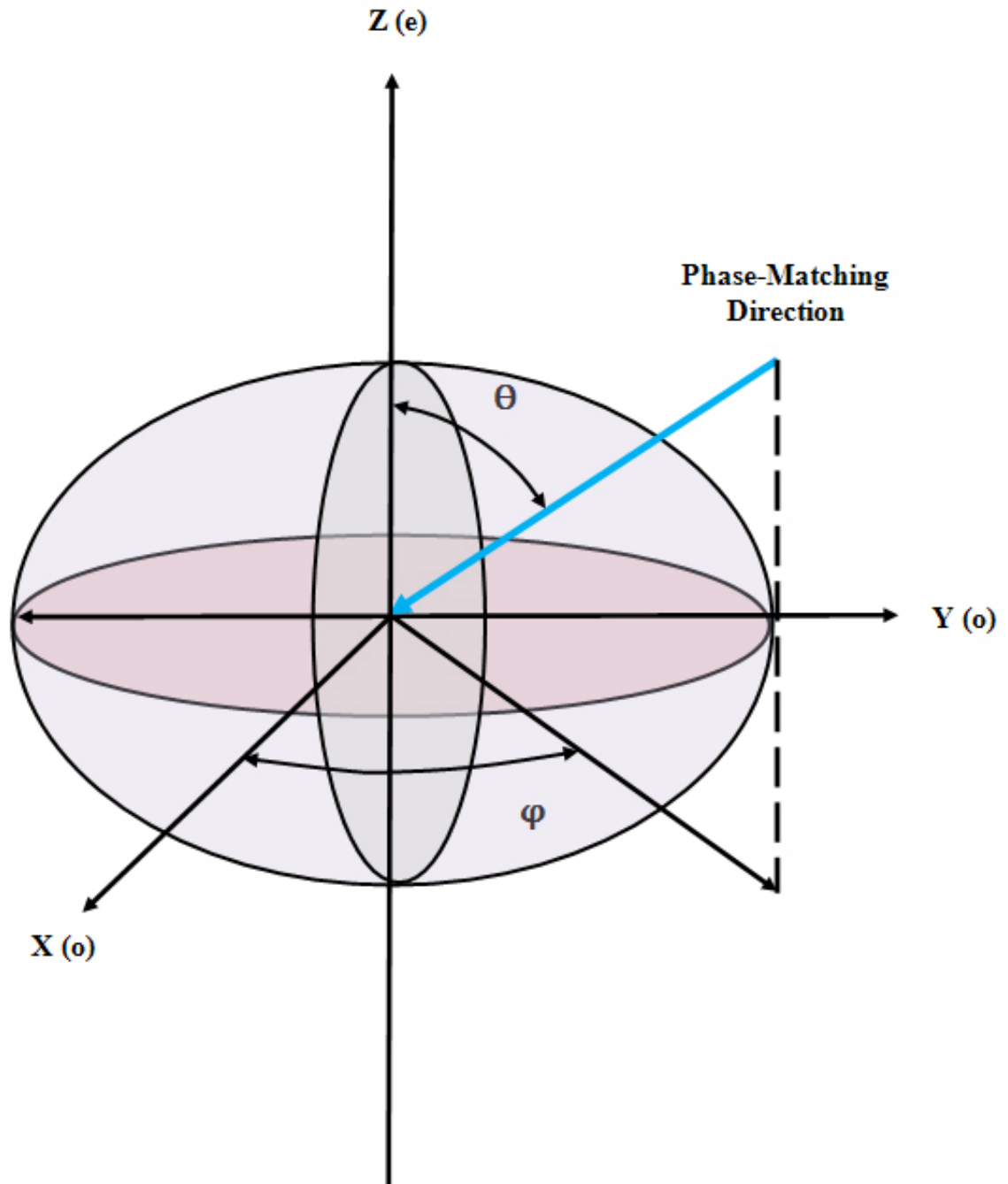


$\text{KBe}_2\text{BO}_3\text{F}_2$ (KBBF) Data Sheet

Potassium Fluoroboratoberyllate

KBBF Crystal Axes and Phase-Matching Direction



Reference:

[1] D. N. Nikogosyan, *Nonlinear Optical Crystals*, Springer (2005)

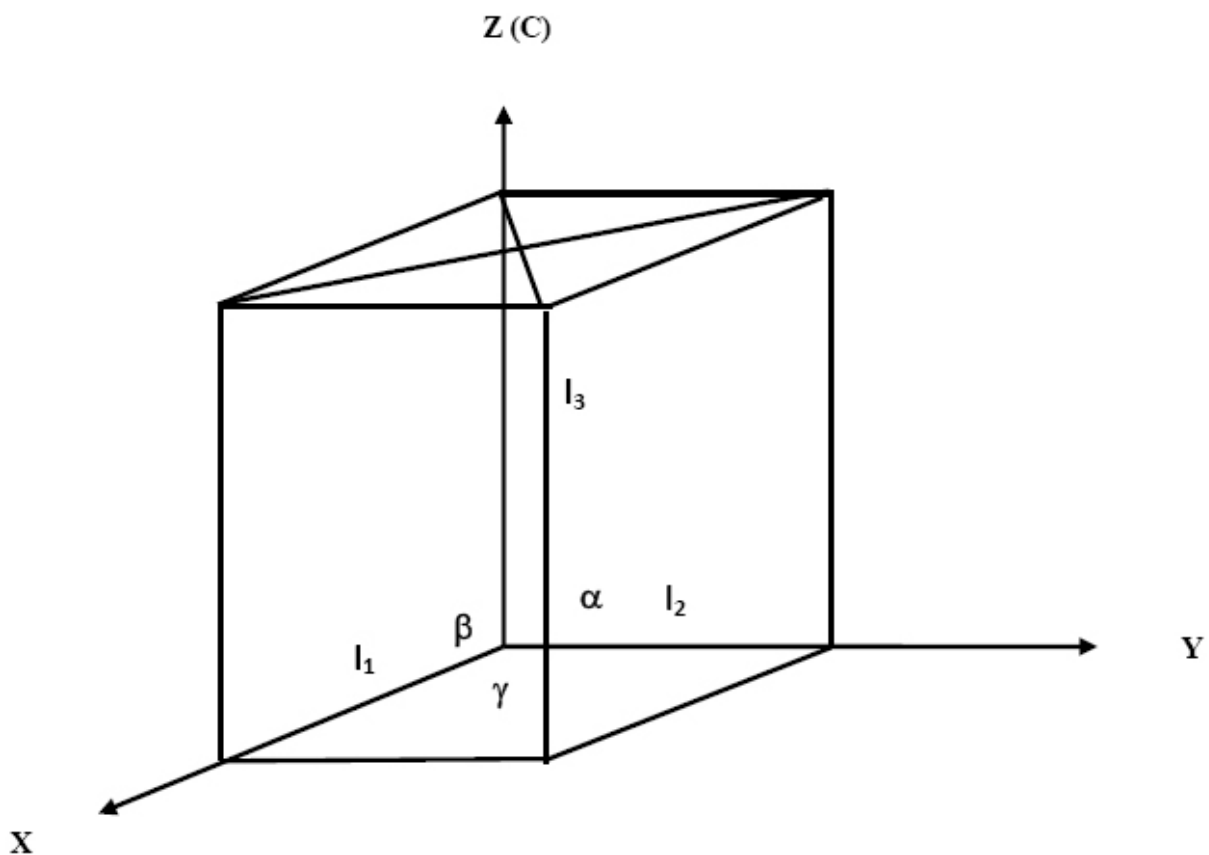
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I. General Properties

(1) Crystal Structure	Class R32 Hexagonal (Trigonal) [1,2,3]
(2) Crystal Optical Class	Negative Uniaxial
(3) Crystal Unit Cell	Hexagonal
(4) Crystal Lattice Constants (A)	$c = 18.734$ $a = 4.442$
(5) Crystal Axes and Unit Cell Conventions	



Right Handed System (X, Y, Z) of Physical Axes

(6) Crystal Unit Cell Length Definitions	$l_1 = l_2 = a, l_3 = c$
(7) Crystal Unit Cell Angle Definitions	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$
(8) Unit Cell Volume	$V = 317.25 \text{ \AA}^3$
(9) Hermann-Mauguin Symbol	R32
(10) Symmetry Elements	$1A_3, 3A_2$

- (11) Formulae/Unit Cell** 1
- (12) Crystal Growth Method** Hydrothermal or Flux
- (13) Crystal Growth Direction** Along C-Axis

(14) References

[1] C.D. McMillen and J. W. Kolis, Jour. Of Crys. Growth 310, 2033-2038 (2008)

[2] D. R. Lovett, Tensor Properties of Crystals, Adam Hilger (1990)

[3] ANSI/IEEE Std 176-1987, IEEE Piezoelectric Standard, The Institute of Electrical and Electronics Engineers, Inc 345 East 47th Street, New York, NY 10017, USA (1988).

II. Optical Properties

(1) Transparency Range

Table 1: Numerical Values for Transparency Range (nm)

References	Transparency Range (nm)
[1]	155 – 3660

(2) Dielectric Matrix and Coefficient Values:

$$\varepsilon = \varepsilon_0 \begin{bmatrix} n_o^2 & 0 & 0 \\ 0 & n_o^2 & 0 \\ 0 & 0 & n_e^2 \end{bmatrix}$$

Here, ε is the permittivity, ε_0 is the permittivity of free space, n_o is the ordinary index of refraction, and n_e is the extraordinary index of refraction.

(3) Indices of Refraction (Experimental, Flux Grown) [2]

Table 2: KBBF Index of Refraction at 295 K

Wavelength (nm)	n_o	n_e
4047	1.4915	1.4035
4358	1.4887	1.4018
4916	1.4851	1.3993
5461	1.4824	1.3976
5780	1.4811	1.3968
5893	1.4808	1.3966
6562	1.4788	1.3954

(4) Sellmeier Equations (Flux Grown) [2]

Table 3: Various Sellmeier Equations Used to Determine Indices of Refraction

Reference	n_o	n_e
[2]	$n_o^2 = 1 + \frac{A\lambda^2}{\lambda^2 - B} - C\lambda^2$	$n_e^2 = 1 + \frac{D\lambda^2}{\lambda^2 - E} - F\lambda^2$

Constant Values: (Expressed in $(1/\mu\text{m}^2)$)

Wavelengths: (Expressed in μm)

Where, $A = 1.1713$ (Dimensionless), $B = 0.00733$ (μm^2), $C = 0.01022$ ($1/\mu\text{m}^2$),
 $D = 0.9316$ (Dimensionless), $E = 0.00675$ (μm^2), $F = 0.00169$ ($1/\mu\text{m}^2$)

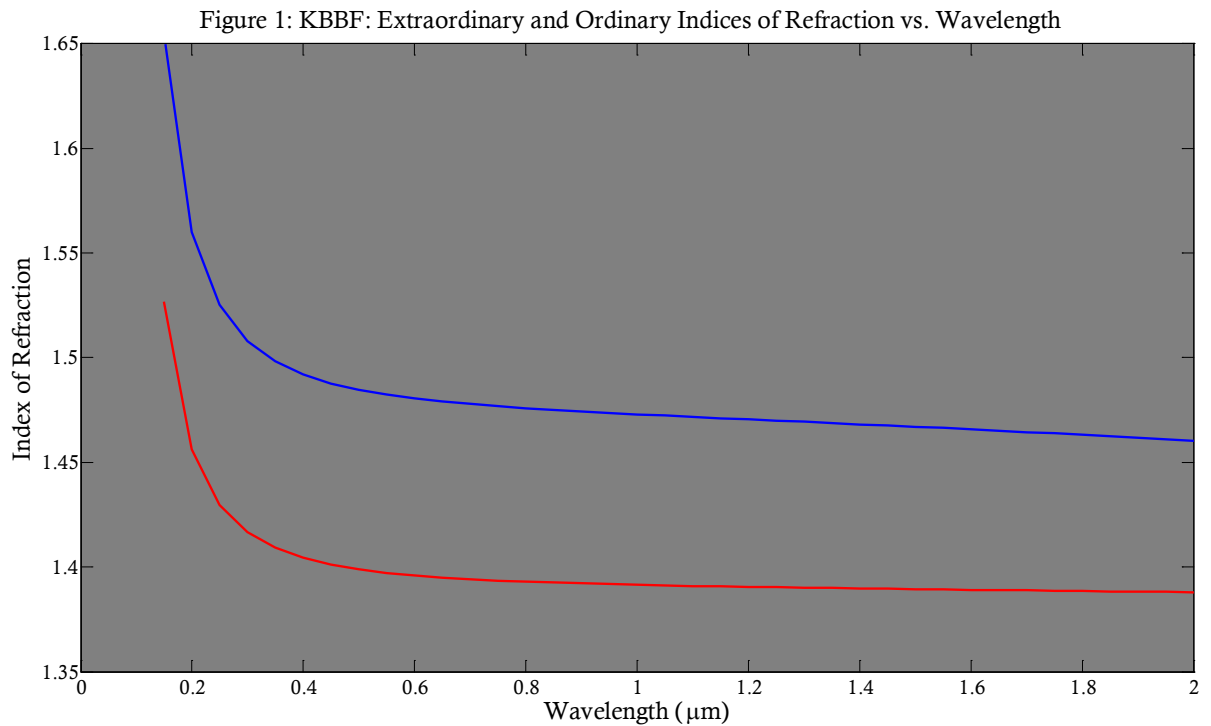


Figure 1: The table below shows the information that was included in the above graph. The data points and Sellmeier equations used are those that were previously defined II.(4).

Table 4: Index of Refraction vs. Wavelength

Reference	n _o (Ordinary Index)	n _e (Extraordinary Index)
[2]	—	—

(5) Selected Index of Refraction Values (Flux Grown) For Second Harmonic Generation (SHG)

Table 5: Numerical Values of Index of Refraction for Second Harmonic Generation (SHG)

Process	Fundamental Wavelength (nm)	Harmonic Wavelength (nm)	$n_o^{\omega} = n_e^{2\omega}$
SHG Nd:YAG	532.00	266.00	1.483
SHG Yb:YAG	514.50	257.25	1.484
SHG Nd:YAG	473.00	236.50	1.486
SHG Nd:YVO ₄	457.00	228.50	1.487
SHG Nd:GdVO ₄	456.00	228.00	1.487

SHG Ti:Al ₂ O ₃	400.00	200.00	1.492
SHG Ti:Al ₂ O ₃	394.00	197.00	1.493
SHG Ti:Al ₂ O ₃	372.60	186.30	1.495
SHG Ti:Al ₂ O ₃	358.70	179.40	1.497

(6) Linear Loss Coefficients

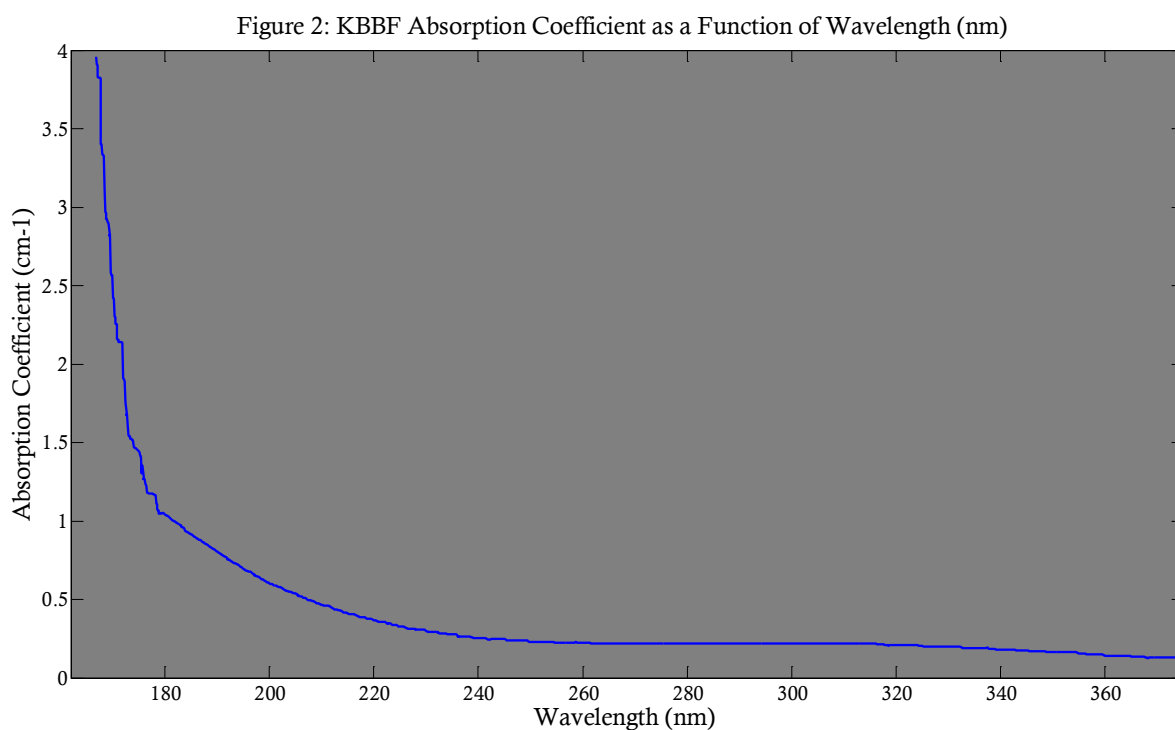


Figure 2: The table below shows the information that was included in the above graph.

Table 6: KBBF Absorption Coefficient vs. Wavelength

Reference	Wavelength (nm)	Absorption Coefficient Value (cm-1)
[3,4]		—
[4]	266.0 nm	0.188
[4]	257.25 nm	0.193
[4]	236.50 nm	0.262

(7) Change in Index of Refraction With Temperature: [5]

(8) Nonlinear Index of Refraction and Nonlinear Coefficient: [5]

(9) Bare Surface KBBF Optical Damage Threshold Values [6,7,8,9,10]

Table 7: Numerical Values for Bare Surface KBBF Optical Damage

Reference	Fluence (J/cm ²)	Intensity (GW/cm ²)	Pulsewidth (FWHM)	Wavelength (nm)	Repetition Rate (Hz)
[6,7]	>40	>5.0	8 ns	1064	Unknown
[8]	>0.147	>4.2	35 ps	532	Unknown
[6]	>0.406	>11.6	35 ps	532	10
[9]	>0.210	>7.0	30 ps	532	Unknown
[10]	> 40	> 40	1 ns	1064	Unknown

(10) References:

[1] V. Petrov, F. Rotermund, F. Noack, J. Ringling, O. Kittelmann, and R. Komatsu, "Frequency conversion of Ti:Sapphire – based femtosecond laser systems to the 200 – nm spectral range using nonlinear optical crystals", IEEE J. of Select. Top. In Quantum. Electron. 5, 1532- 1542 (1999).

[2] C. Chen, G. Wang, X. Wang, Y. Zhu, Z. Xu, T. Kanai, and S. Watanabe, "Improved Sellmeier equations and phase-matching characteristics in deep-ultraviolet region of KBe₂BO₃F₂ crystal", IEEE J. Quantum. Electron. 44, 617-621 (2008).

[3] B. Wu, D. Tang, N. Ye, and C. Chen, "Linear and nonlinear optical properties of the KBe₂BO₃F₂ (KBBF) crystal", Opt. Materials 5, 105-109 (1996).

[4] Z. Wang, J. Zhang, F. Yang, X. Cheng, Y. Zhou, J. Xu, Y. Xu, Y. Bo, Q. Peng, D. Cui, Z. Xu, X. Wang, Y. Zhu, and C. Chen, "Stable operation of 4 mW nanoseconds radiation at 177.3 nm by second harmonic generation in KBe₂BO₃F₂ crystals", Opt. Express 17, 20021 – 20032 (2009).

[5] No Measurements Reported

[6] J. Lu, G. Wang, Z. Xu, C. Chen, J. Wang, C. Zhang, and Y. Liu, "High-efficiency fourth-harmonic generation of KBBF crystal", Opt. Commun. 200, 415-418 (2001).

[7] C. Chen, J. Lu, G. Wang, Z. Xu, J. Wang, C. Zhang, and Y. Liu, "Deep ultraviolet harmonic generation with KBe₂BO₃F₂ crystal", Chin. Phys. Lett. 18, 1081 (2001)

[8] G., Wang, C. Zhang, C. Chen, A. Yao, J. Zhang, Z. Xu, and J. Wang, "High-efficiency 266-nm output of a KBe₂BO₃F₂ crystal", Appl. Opt. 42, 4331-4334 (2003).

[9] B. Wu, D. Tang, N. Ye, and C. Chen, "Linear and nonlinear optical properties of the KBe₂BO₃F₂ (KBBF) crystal", Opt. Materials 5, 105-109 (1996).

[10] P. Kumbhakar, T. Kobayashi, "Ultra-broadband optical parametric amplification in KBe₂BO₃F₂ crystal", Opt. Commun. 277, 205-208 (2007).

III. Nonlinear Properties

(1) Effective Second-Order Nonlinear Coefficient

Assumes Kleinman symmetry conditions are valid.

Type I Phase-Matching:

$$d_{\text{eff}} = d_{\text{ooe}} = d_{11} \cdot \cos(\theta) \cdot \cos(3\varphi)$$

Type II Phase-Matching:

$$d_{\text{eff}} = d_{\text{eoc}} = d_{\text{oc e}} = d_{11} \cdot \cos^2(\theta) \cdot \sin(3\varphi)$$

Absolute Value of d_{11} : $d_{11} = 0.49 \text{ pm/V}$ [1]

(2) Variation of Second-Order Nonlinear Coefficient With Phase-Matching Angle

**Table 8: Numerical Values for Type 1 (ooe)
Second-Order Nonlinear Coefficient With Phase-Matching Angle**

Phase Matching Angle Theta (Degrees)	d_{eff} (pm/V)
15	0.473
20	0.460
25	0.444
30	0.424
35	0.401
40	0.375
45	0.346
50	0.315
55	0.281
60	0.245
65	0.207
70	0.168
75	0.127

**Table 9: Numerical Values for Type 2 (eoe or oee)
Second-Order Nonlinear Coefficient With Phase-Matching Angle**

Phase Matching Angle Theta (Degrees)	d_{eff} (pm/V)
15	0.457
20	0.433
25	0.402
30	0.368

35	0.329
40	0.288
45	0.245
50	0.202
55	0.161
60	0.123
65	0.088
70	0.057
75	0.033

Figure 3: d_{eff} as a Function of Phase-Matching Angle Θ

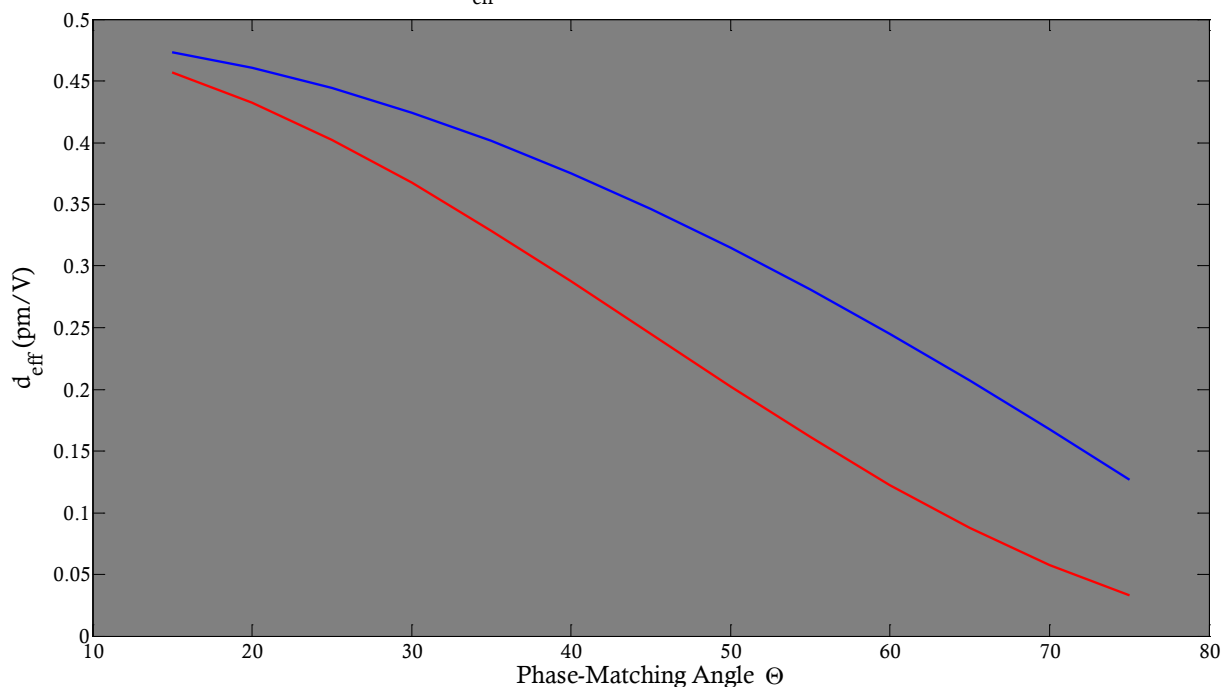


Figure 3: The table below shows the information that was included in the above graph. The data points used are those that were previously defined III.(2).

Table 10: Phase-Matching Angle θ vs. Second Order Nonlinear Coefficient d_{eff}

Reference	Type I	Type II
[2]		

(3) Calculated Values of Critical Phase-Matching Angles [2]

Table 11: Numerical Calculated Values for Critical Phase-Matching Angles

Fundamental Wavelength (μm)	Phase-Matching Angle (Degrees)
1.4000	19.06
1.3420	19.02
1.3000	19.04

1.2000	19.27
1.0640	20.10
1.0290	20.43
0.9500	21.41
0.9000	22.20
0.8500	23.17
0.7700	25.16
0.6800	28.23
0.6000	32.07
0.5890	32.70
0.5500	35.25
0.5320	36.60
0.5145	38.04
0.5000	39.34
0.4800	41.32
0.4760	41.74
0.4600	43.56
0.4400	46.14
0.4100	50.82
0.3847	55.91
0.3743	58.46
0.3685	60.04
0.3884	55.08
0.3786	57.37
0.3674	60.35
0.3644	61.24
0.3612	62.23
0.3547	64.42
0.3524	65.26
0.3450	68.27
0.3400	70.66

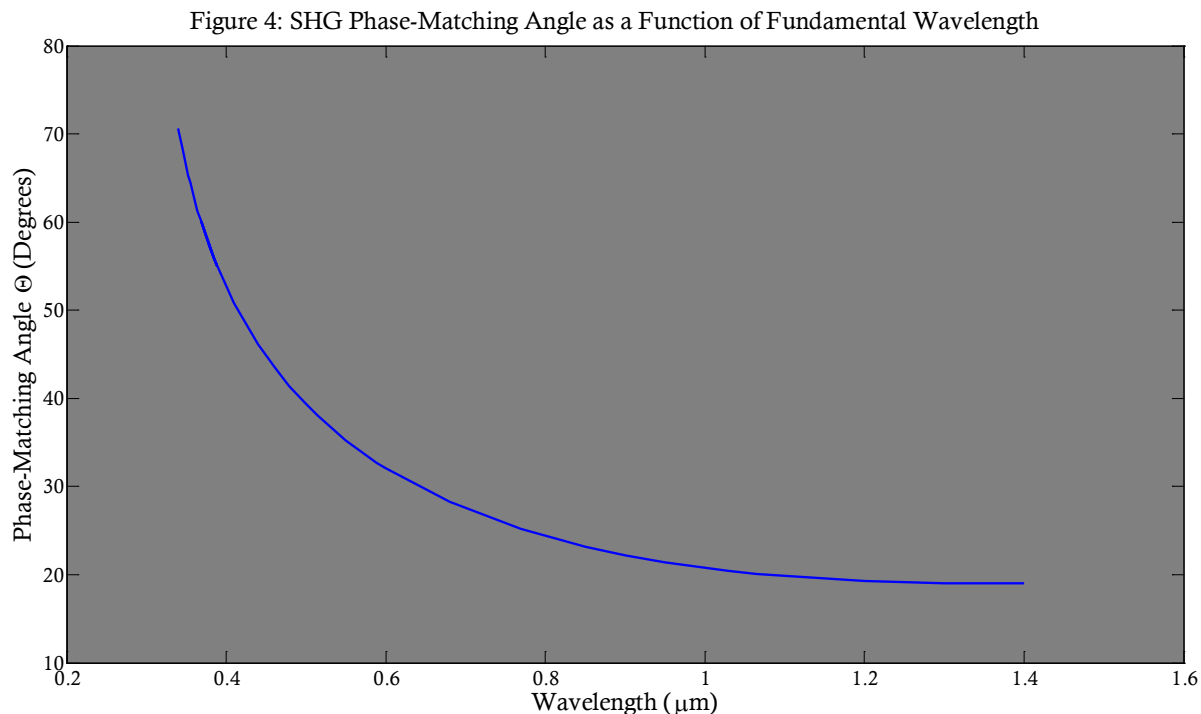


Figure 4: The table below shows the information that was included in the above graph. The data points used are those that were previously defined III.(3).

Table 12: Critical Phase-Matching Angles vs. Fundamental Wavelength

Reference	Phase Matching Angle
[2]	—

(4) Measured Values of Critical Phase-Matching Angles [3]

Table 13: Numerical Measured Values for Critical Phase-Matching Angles

Interacting Wavelength (nm)	Measured Phase-Matching Angle (Degrees)
$345(o)+345(o)=172.5(e)$	71.0
$354.6(o)+354.6(o)=177.3(e)$	66.2
$369.5(o)+369.5(o)=184.75(e)$	61.0
$374.3(o)+374.3(o)=187.15(e)$	59.4
$384.7(o)+384.7(o)=192.35(e)$	56.8
$410(o)+410(o)=205(e)$	51.5
$440(o)+440(o)=220(e)$	46.0
$460(o)+460(o)=230(e)$	44.0
$480(o)+490(o)=240(e)$	41.7
$500(o)+500(o)=250(e)$	39.6
$532(o)+532(o)=266(e)$	36.2
$550(o)+550(o)=275(e)$	34.9

589(o)+589(o)=294.5(e)	32.5
600(o)+600(o)=300(e)	32.1
680(o)+680(o)=340(e)	27.6
770(o)+770(o)=385(e)	25.1
850(o)+850(o)=425(e)	23.1
900(o)+900(o)=450(e)	22.0
950(o)+950(o)=475(e)	21.0
1064(o)+1064(o)=532(e)	20.2
1342(o)+1342(o)=671(e)	18.6

(5) Walk-Off Angles ρ_w and Wave Mismatch Sensitivities For Selected SHG Processes [4]

In negative uniaxial crystals the walkoff angle ρ_w is positive ($\rho_w > 0$), and can be calculated from

$$\rho_w = \tan^{-1} \left(\left(\frac{n_o^2}{n_e^2} \right) \tan(\theta) \right) - \theta$$

Table 14: Numerical Values for Walk-Off Angles ρ_w and Wave Mismatch Sensitivities For Selected SHG Processes

SHG Process (Wavelengths in nm)	ρ_w^{ω} (mrad)	$\rho_w^{2\omega}$ (mrad)	θ Sensitivity (mrad-cm)	Temperature Sensitivity (°C-cm)	Spectral Sensitivity (mm-cm)
532(o)+532(o)=266(e)	0.00	62.14	0.29	Unknown	Unknown
514.5(o)+514.5(o)=257.25(e)	0.00	63.23	0.27	Unknown	Unknown
473(o)+473(o)=236.5(e)	0.00	65.45	0.24	Unknown	Unknown
400(o)+400(o)=200(e)	0.00	65.07	0.21	Unknown	Unknown
380(o)+380(o)=190(e)	0.00	62.21	0.20	Unknown	Unknown
360(o)+360(o)=180(e)	0.00	56.27	0.21	Unknown	Unknown
340(o)+340(o)=170(e)	0.00	43.62	0.26	Unknown	Unknown

(6) References

[1] C. Chen, Z. Lin, Z. Wang, “The development of new borate based UV nonlinear crystals”, App. Phys. B 80, 1-25 (2005).

[2] C. Chen, G. Wang, X. Wang, Y. Zhu, Z. Xu, T. Kanai, and S. Watanabe, “Improved Sellmeier equations and phase-matching characteristics in deep-ultraviolet region of $\text{KBe}_2\text{BO}_3\text{F}_2$ crystal”, IEEE J. Quantum. Electron. 44, 617-621 (2008).

[3] D. N. Nikogosyan, Nonlinear Optical Crystals, Springer (2005)

[4] Calculated Using Sandia Nonlinear Optics Program (www.as-photonics.com/SNLO).

IV. Mechanical Properties

(1) Mass Density ρ (gr/cm³) at 295 K

Table 15: Numerical Values of Mass Density ρ (gr/cm³) at 295 K

Reference	ρ (gr/cm ³)
[1] Calculated	4.550

(2) Molecular Weight w_m (gm)

Table 16: Numerical Values for Molecular Weight w_m (gm)

Reference	w_m
[1]	153.93 gr

(3) Mohs Hardness: [2]

(4) Compliance Matrix s (cm²/kgm) (Rank 4)

$$s = \begin{bmatrix} s_{11} & s_{12} & s_{13} & s_{14} & 0 & 0 \\ s_{12} & s_{11} & s_{13} & -s_{14} & 0 & 0 \\ s_{13} & s_{13} & s_{33} & 0 & 0 & 0 \\ s_{14} & -s_{14} & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 2s_{14} \\ 0 & 0 & 0 & 0 & 2s_{14} & 2(s_{11} - s_{12}) \end{bmatrix}$$

(5) Elastic Stiffness Matrix c (GPa or kgm/cm²) (Rank 4)

$$c = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ c_{12} & c_{11} & c_{13} & -c_{14} & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & 0 & c_{14} & 1/2(c_{11} - c_{12}) \end{bmatrix}$$

(6) Poisson's Ratio ν : [2]

(7) Young's Modulus E : [2]

(8) References:

[1] C. D. McMillan and J. W. Kolis, "Hydrothermal crystal growth of $ABe_2BO_3F_2$ (A= K, Rb, Cs, Tl) NLO Crystals", J. of Crys. Growth 310, 2033-2039 (2008).

[2] No Measurements Reported.

VII. Thermal Properties

(1) Debye Temperature Θ_D : [1]

(2) Melting Temperature T_m (K):

Table 17: Numerical Values for Melting Temperature T_m (K)

Reference	T_m (K)
[2] (Flux Grown)	<800 °C

(3) Thermal Conductivity Matrix and Coefficient Values k (W/(cm-K))

$$k = \begin{bmatrix} k_{11} & 0 & 0 \\ 0 & k_{22} & 0 \\ 0 & 0 & k_{33} \end{bmatrix} = \begin{bmatrix} k_a & 0 & 0 \\ 0 & k_a & 0 \\ 0 & 0 & k_c \end{bmatrix}$$

Using the axes convention shown previously, here we have $k_{11} = k_{22} = k_a = k_b$, and $k_{33} = k_c$ where a, b, and c refer to the crystalline axes and thermal conductivity is parallel to specified axis.

Table 18: Numerical Values of k (W/(cm-K)) at 298 K

Reference	k W/cm-K
[3] Axis Not Specified	0.0025

(4) Thermal Expansion Matrix and Coefficient Values α (1/K) [1]

$$\alpha = \begin{bmatrix} \alpha_{11} & 0 & 0 \\ 0 & \alpha_{22} & 0 \\ 0 & 0 & \alpha_{33} \end{bmatrix} = \begin{bmatrix} \alpha_a & 0 & 0 \\ 0 & \alpha_a & 0 \\ 0 & 0 & \alpha_c \end{bmatrix}$$

Using the axes convention shown previously, here we have $\alpha_{11} = \alpha_{22} = \alpha_a = \alpha_b$, and $\alpha_{33} = \alpha_c$, where a, b, and c refer to the crystal axes and the thermal expansion coefficient is parallel to specified axis.

(5) Specific Heat c_p (J/(gr-K)): [1]

(6) References:

[1] No Measurements Reported

[2] C. D. McMillan and J. W. Kolis, "Hydrothermal crystal growth of $ABe_2BO_3F_2$ (A= K, Rb, Cs, Tl) NLO Crystals", J. of Crys. Growth 310, 2033-2039 (2008).

[3] C. Chen, Z. Lin, Z. Wang, "The development of new borate based UV nonlinear crystals", App. Phys. B 80, 1-25 (2005).