Supporting Information

UV Nonlinear Optical Crystals: Alkaline Beryllium Borate $NaBeB_3O_6$ and $ABe_2B_3O_7$ (A = K, Rb)

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Table S1. Atomic Positions and Isotropic Displacement Factors for $NaBeB_3O_6$

atom	x	y	z	Wyckoff	$U_{eq}(Å^2)$	occupancy
Na	0.67295(11)	0.38903(9)	0.2748(3)	4a	0.0284(3)	1
Be	0.9084(3)	0.4573(3)	-0.1701(8)	4a	0.0145(7)	1
B(1)	0.9309(3)	0.2446(2)	-0.1194(7)	4a	0.0156(6)	1
B(2)	0.5839(3)	0.1641(2)	0.5005(7)	4a	0.0154(6)	1
B(3)	0.7783(3)	0.1038(2)	0.1607(7)	4a	0.0153(6)	1
O(1)	0.88438(17)	0.33995(14)	-0.0019(4)	4a	0.0159(4)	1
O(2)	0.52980(18)	0.25971(14)	0.6370(5)	4a	0.0199(4)	1
O(3)	0.53778(16)	0.05886(13)	0.5668(4)	4a	0.0142(4)	1
O(4)	0.69571(17)	0.18778(14)	0.2990(4)	4a	0.0194(4)	1
O(5)	0.75483(16)	0.49623(13)	0.6835(5)	4a	0.0178(4)	1
O(6)	0.39676(18)	0.36262(14)	-0.0171(4)	4a	0.0209(5)	1

Table S2. Atomic Positions and Isotropic Displacement Factors for α-$KBe_2B_3O_7$

atom	x	y	z	Wyckoff	$U_{eq}(Å^2)$	occupancy
K	0	0.17903(5)	0.25	4e	0.0143(2)	1
Be	0.15472(19)	0.2094(2)	-0.1573(3)	8f	0.0083(4)	1
B(1)	0	0.4496(3)	-0.25	4e	0.0101(5)	1
B(2)	0.24832(17)	0.01919(17)	0.1830(3)	8f	0.0081(4)	1
O(1)	0	0.29746(15)	-0.25	4e	0.0083(3)	1
O(2)	0.22101(11)	0.16540(10)	0.11682(17)	8f	0.0078(3)	1
O(3)	0.38608(11)	-0.03378(11)	0.2360(2)	8f	0.0143(3)	1
O(4)	0.15051(11)	-0.07066(11)	0.19650(18)	8f	0.0106(3)	1

Table S3. Atomic Positions and Isotropic Displacement Factors for β-$KBe_2B_3O_7$

atom	x	y	z	Wyckoff	$U_{eq}(Å^2)$	occupancy
K(1)	0.5	0.63740(4)	0.60735(16)	2a	0.02217(17)	1
K(2)	1	0.85304(4)	0.67704(16)	2a	0.0270(2)	1
Be(1)	0.8114(3)	0.54184(12)	1.1265(6)	4b	0.0082(4)	1
Be(2)	0.6760(3)	0.96271(13)	1.2717(6)	4b	0.0091(4)	1
B(1)	1	0.51993(14)	1.6236(8)	2a	0.0070(5)	1
B(2)	0.5	0.99094(16)	0.7656(7)	2a	0.0070(5)	1
B(3)	0.8397(3)	0.68439(13)	1.0455(5)	4b	0.0152(5)	1
B(4)	0.6653(3)	0.80692(12)	1.1722(7)	4b	0.0205(5)	1
O(1)	1	0.52718(10)	1.3114(4)	2a	0.0092(4)	1
O(2)	0.84267(14)	0.51336(7)	0.7755(3)	4b	0.0086(3)	1
O(3)	0.5	0.99116(10)	1.4518(4)	2a	0.0099(4)	1
O(4)	0.65529(15)	0.99270(8)	0.9196(3)	4b	0.0110(3)	1
O(5)	0.73767(16)	0.62808(6)	1.1379(4)	4b	0.0133(3)	1
O(6)	1	0.66921(10)	0.9056(5)	2a	0.0162(4)	1
O(7)	0.8026(2)	0.76114(8)	1.0715(6)	4b	0.0457(7)	1
O(8)	0.5	0.77556(11)	1.1303(8)	2a	0.0311(5)	1
O(9)	0.70627(18)	0.87378(7)	1.2860(4)	4b	0.0198(3)	1

Table S4. Atomic Positions and Isotropic Displacement Factors for γ-$KBe_2B_3O_7$

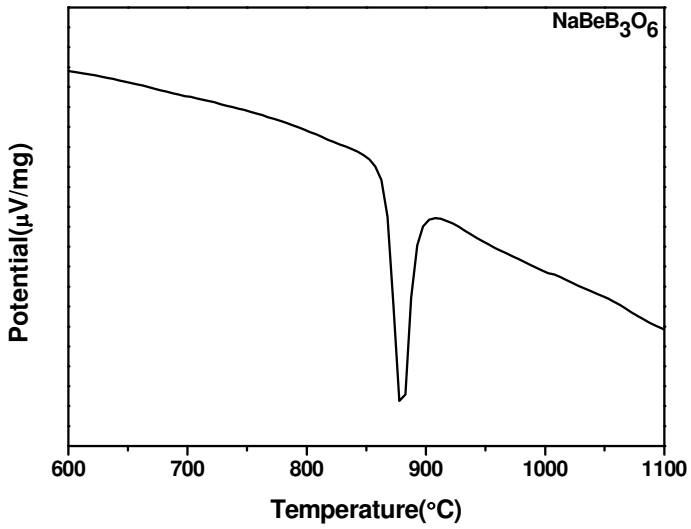
atom	x	y	z	Wyckoff	U_{eq}(Å^2)	occupancy
K(1)	0.36979(18)	0.55848(7)	0.76653(12)	2a	0.0219(3)	1
K(2)	0.37906(17)	0.91092(7)	0.76614(13)	2a	0.0201(3)	1
K(3)	0.0018(3)	0.48280(13)	1.0054(2)	2a	0.0364(3)	1
Be(1)	-0.0238(9)	0.3960(3)	0.5867(7)	2a	0.0075(11)	1
Be(2)	0.0308(8)	0.5626(4)	0.4230(6)	2a	0.0081(11)	1
Be(3)	0.3969(8)	0.5634(4)	0.4157(6)	2a	0.0081(11)	1
Be(4)	0.6001(9)	0.3954(3)	0.5781(6)	2a	0.0092(12)	1
Be(5)	0.3988(6)	0.2275(5)	0.4084(5)	2a	0.0082(8)	1
Be(6)	0.0277(6)	0.2304(5)	0.4107(5)	2a	0.0074(8)	1
B(1)	0.2361(8)	0.3961(3)	0.4638(6)	2a	0.0102(11)	1
B(2)	0.2359(5)	0.7289(4)	0.4737(4)	2a	0.0067(7)	1
B(3)	-0.2339(7)	0.5650(3)	0.5389(5)	2a	0.0058(9)	1
B(4)	0.3445(8)	0.6439(4)	0.1520(6)	2a	0.0149(10)	1
B(5)	0.1912(5)	0.7375(5)	-0.0875(4)	2a	0.0144(8)	1
B(6)	0.3578(7)	0.8237(4)	0.1575(5)	2a	0.0105(9)	1
B(7)	0.3111(5)	0.2282(5)	0.0879(4)	2a	0.0135(8)	1
B(8)	0.1560(8)	0.3227(4)	-0.1495(6)	2a	0.0157(11)	1
B(9)	0.1590(8)	0.1415(4)	-0.1569(6)	2a	0.0188(12)	1
O(1)	-0.0809(3)	0.5123(2)	0.5271(3)	2a	0.0090(5)	1
O(2)	0.0864(4)	0.34526(19)	0.4822(3)	2a	0.0091(5)	1
O(3)	0.2208(3)	0.16531(18)	0.4306(3)	2a	0.0087(5)	1
O(4)	0.3945(3)	0.34626(19)	0.4625(3)	2a	0.0085(5)	1
O(5)	0.6017(3)	0.5121(2)	0.5169(3)	2a	0.0087(5)	1
O(6)	0.2283(3)	0.49909(18)	0.4528(3)	2a	0.0084(5)	1
O(7)	0.3972(3)	0.67712(19)	0.4821(3)	2a	0.0077(5)	1
O(8)	0.0923(3)	0.67583(19)	0.4966(3)	2a	0.0075(5)	1
O(9)	0.2277(3)	0.83195(19)	0.4534(3)	2a	0.0089(5)	1
O(10)	0.1123(4)	0.7407(3)	-0.2358(3)	2a	0.0187(6)	1
O(11)	0.2335(5)	0.6468(2)	-0.0059(4)	2a	0.0168(8)	1
O(12)	0.2441(6)	0.8272(3)	-0.0002(4)	2a	0.0195(8)	1
O(13)	0.3562(6)	0.5613(2)	0.2331(4)	2a	0.0131(7)	1
O(14)	0.4393(4)	0.7320(3)	0.2146(3)	2a	0.0194(6)	1
O(15)	0.3765(6)	0.9044(2)	0.2445(4)	2a	0.0148(8)	1
O(16)	0.3992(4)	0.2256(3)	0.2367(3)	2a	0.0154(6)	1
O(17)	0.2693(5)	0.1400(3)	-0.0005(4)	2a	0.0181(8)	1
O(18)	0.2648(6)	0.3213(2)	0.0076(4)	2a	0.0202(9)	1
O(19)	0.1074(5)	0.0597(2)	-0.2426(4)	2a	0.0127(7)	1
O(20)	0.0830(6)	0.2331(4)	-0.2145(3)	2a	0.0630(13)	1
O(21)	0.1083(6)	0.4061(2)	-0.2311(4)	2a	0.0132(7)	1

Table S5. Atomic Positions and Isotropic Displacement Factors for $RbBe_2B_3O_7$

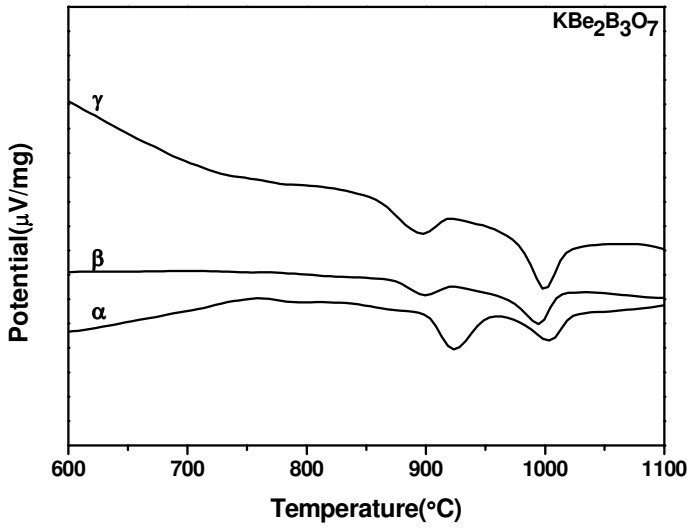
atom	x	y	z	Wyckoff	$U_{eq}(Å^2)$	occupancy
Rb(1)	1	0.64218(3)	0.44656(12)	2a	0.0179(2)	1
Rb(2)	1.5	0.85076(3)	0.42415(15)	2a	0.0210(2)	1
Be(1)	0.6871(6)	0.5402(3)	0.9290(16)	4b	0.0093(10)	1
Be(2)	0.8256(7)	0.9632(3)	0.8578(12)	4b	0.0091(12)	1
B(1)	0.5	0.5190(3)	0.434(2)	2a	0.0063(12)	1
B(2)	1	0.9912(4)	0.3606(15)	2a	0.0075(15)	1
B(3)	0.6588(7)	0.6825(3)	1.0173(12)	4b	0.0165(14)	1
B(4)	0.8367(6)	0.8065(3)	0.9279(18)	4b	0.0182(11)	1
O(1)	0.5	0.5263(2)	0.7440(9)	2a	0.0097(9)	1
O(2)	0.6566(3)	0.51255(16)	1.2819(7)	4b	0.0088(7)	1
O(3)	1	0.9895(2)	0.6743(10)	2a	0.0093(9)	1
O(4)	0.6550(3)	1.00622(17)	0.7083(7)	4b	0.0085(6)	1
O(5)	0.7571(4)	0.62598(14)	0.9224(9)	4b	0.0133(6)	1
O(6)	0.5	0.6690(3)	1.1603(11)	2a	0.0164(10)	1
O(7)	0.6977(4)	0.75778(16)	0.9895(14)	4b	0.0433(13)	1
O(8)	1	0.7740(2)	0.9574(14)	2a	0.0237(10)	1
O(9)	0.7955(4)	0.87553(18)	0.8501(8)	4b	0.0187(8)	1

Table S6. ICP Elemental Analysis and Stoichiometry for $NaBeB_3O_6$ and $ABe_2B_3O_7$ (A = K, Rb)

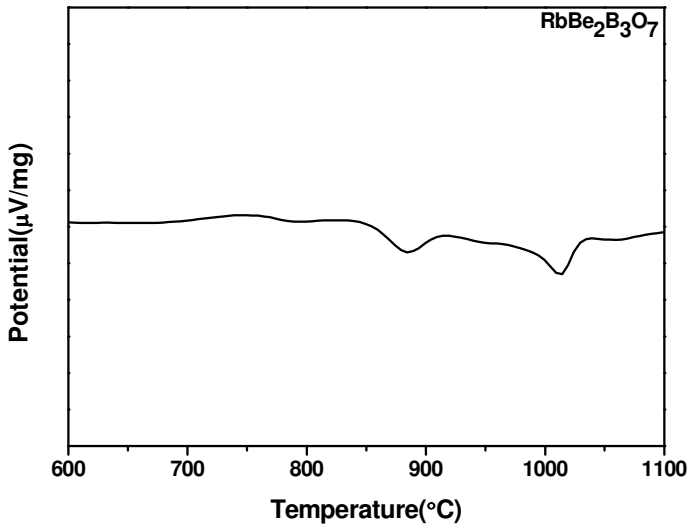
	Na	K	Rb	Be	B
$NaBeB_3O_6$	1			0.96	3.08
α-$KBe_2B_3O_7$		1.12		1.94	3
β-$KBe_2B_3O_7$		1		2.11	2.99
γ-$KBe_2B_3O_7$		1.06		2	2.91
$RbBe_2B_3O_7$			0.96	2	3.02



a. DTA trace for the compositions of $NaBeB_3O_6$

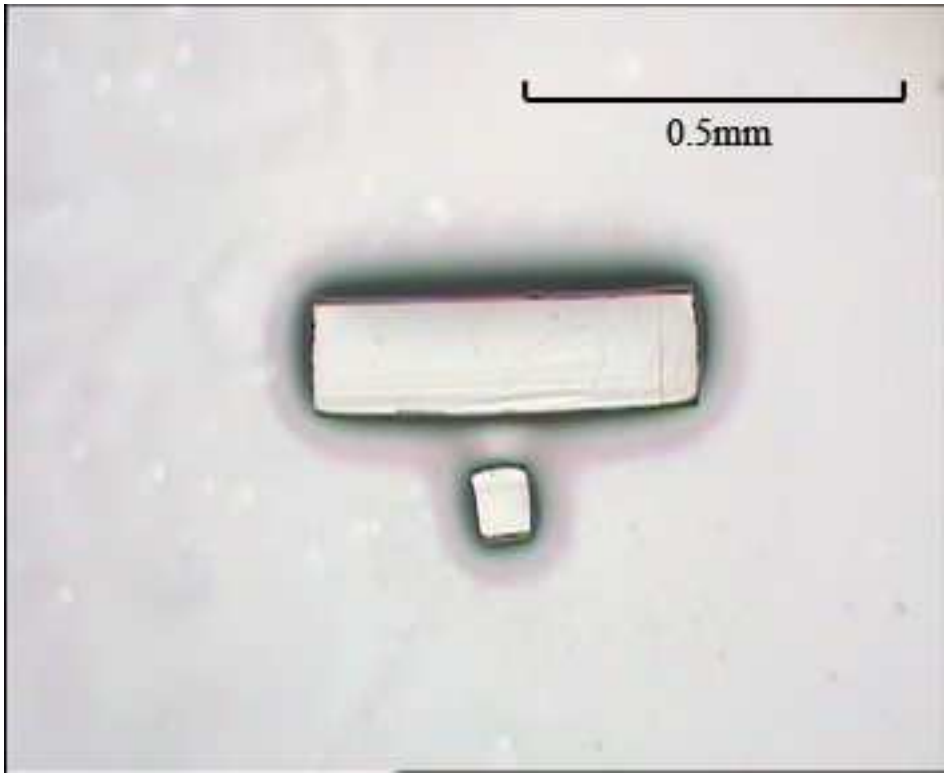


b. DTA trace for the compositions of $KBe_2B_3O_7$

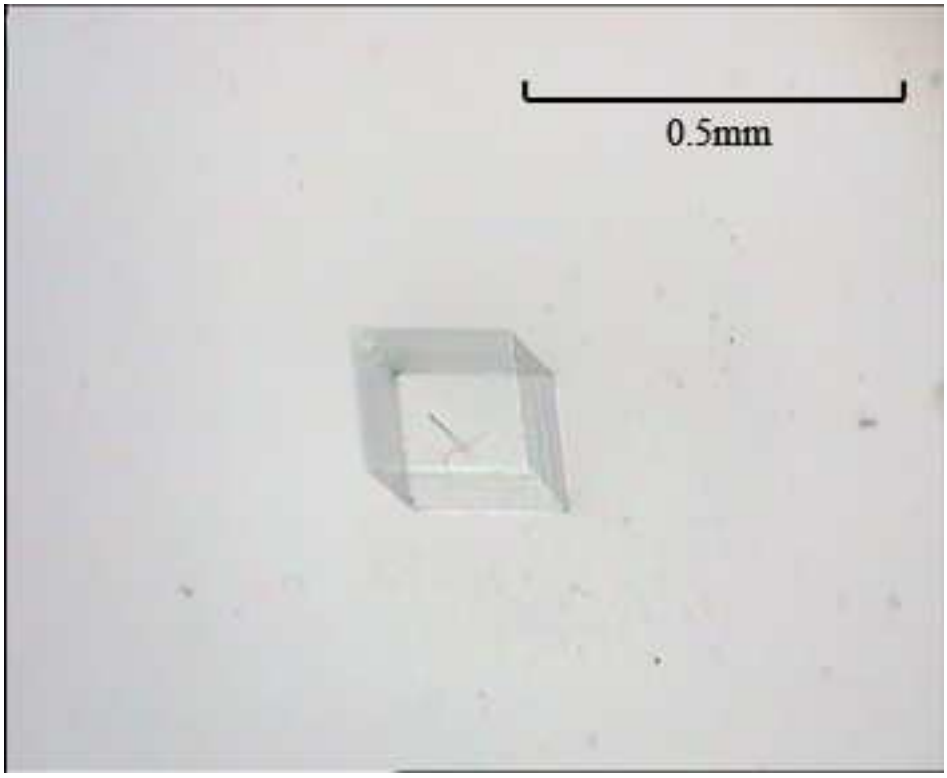


c. DTA trace for the compositions of $RbBe_2B_3O_7$

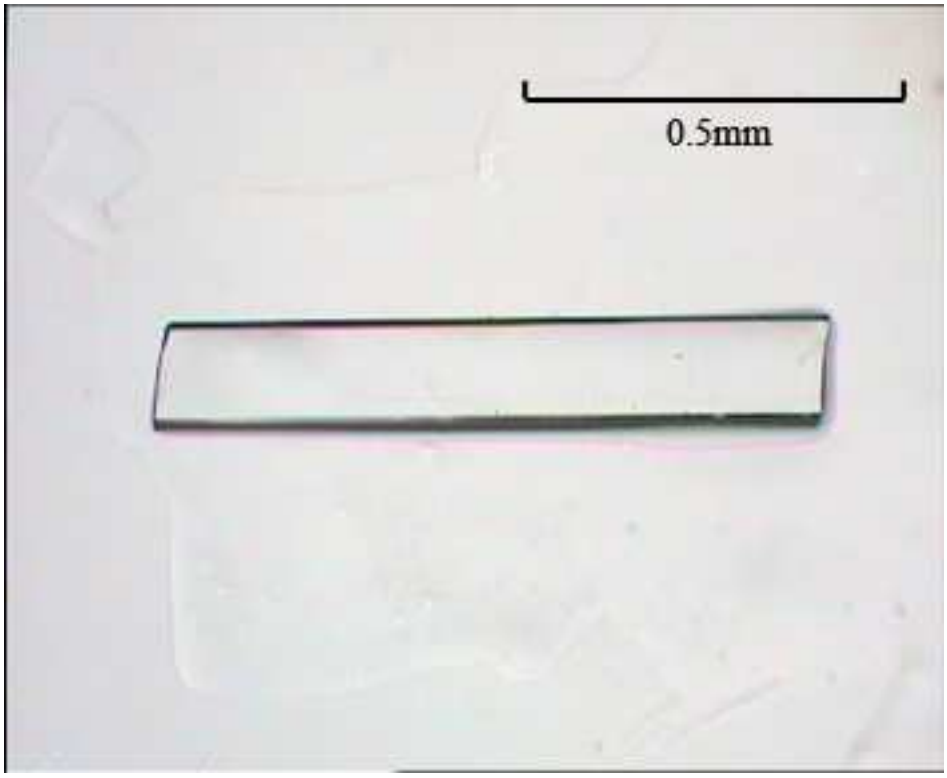
Figure S1. DTA trace for the compositions of $NaBeB_3O_6$ and $ABe_2B_3O_7$ (A = K, Rb)



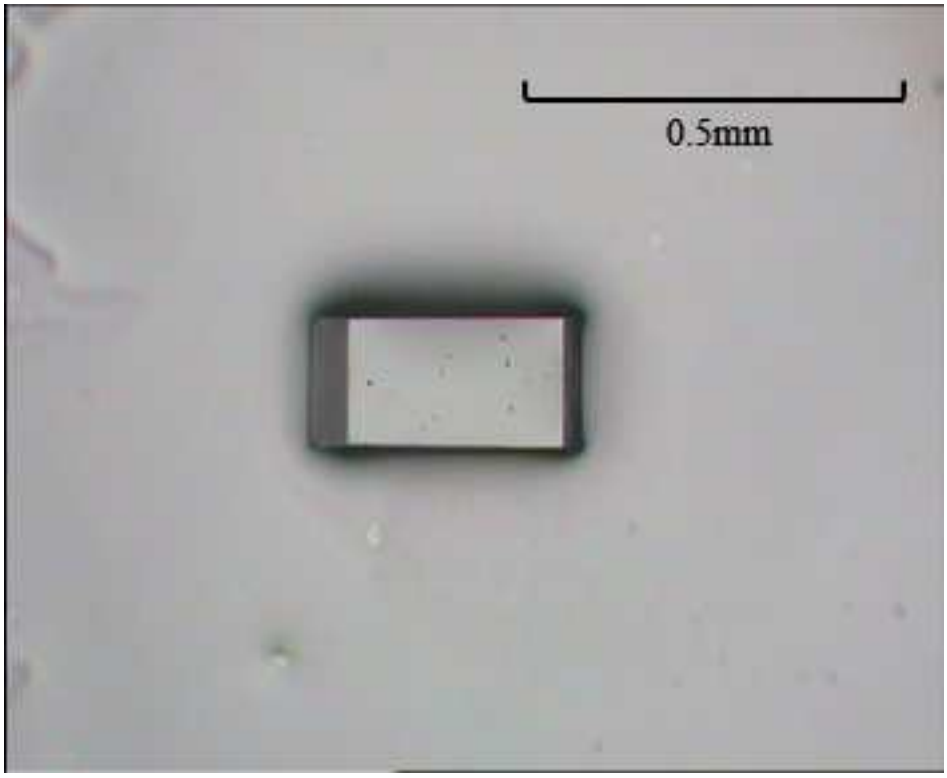
a. As-grown $NaBeB_3O_6$ crystal



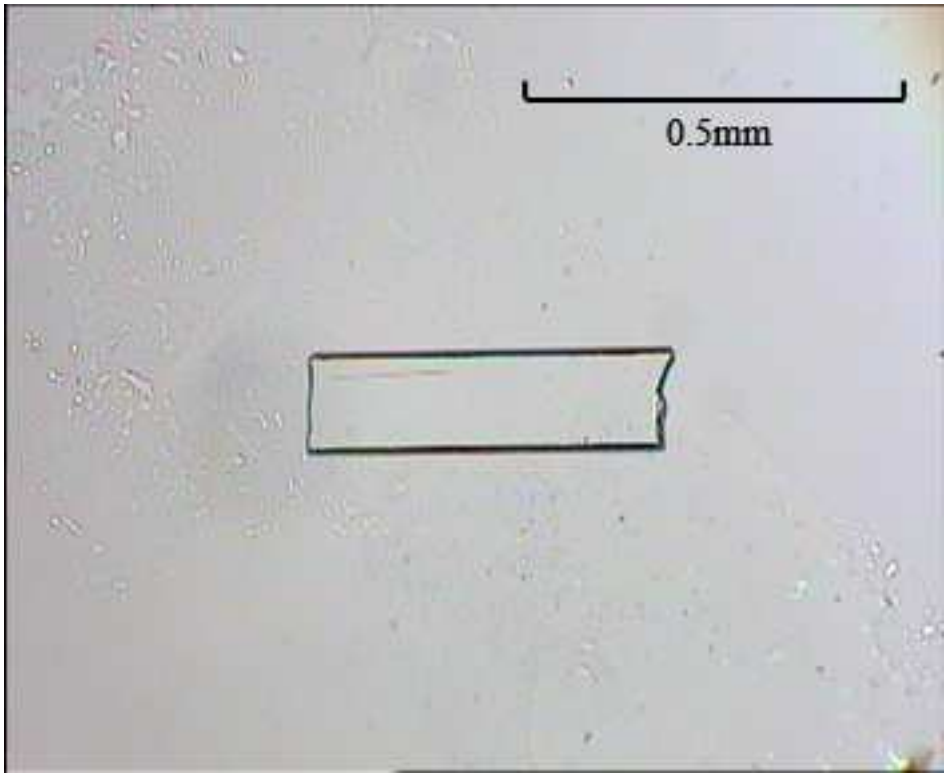
b. As-grown α-$KBe_2B_3O_7$ crystal



c. As-grown β-$KBe_2B_3O_7$ crystal

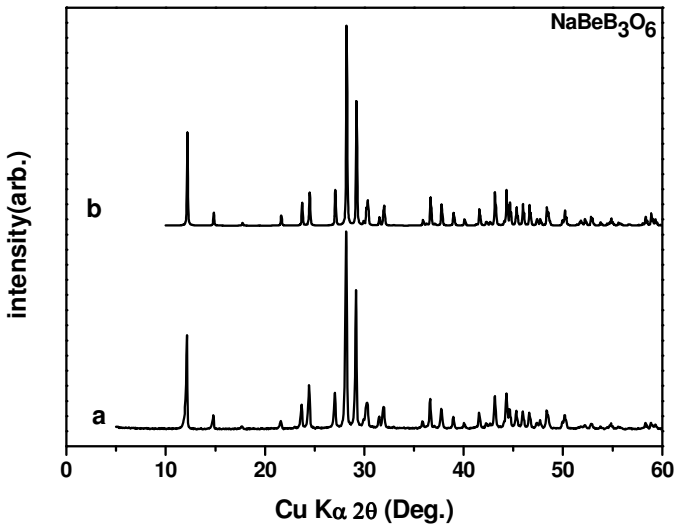


d. As-grown γ-$KBe_2B_3O_7$ crystal

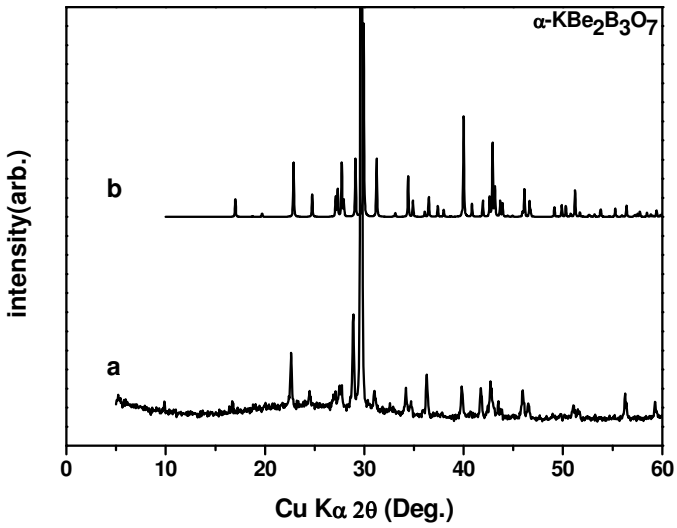


e. As-grown $RbBe_2B_3O_7$ crystal

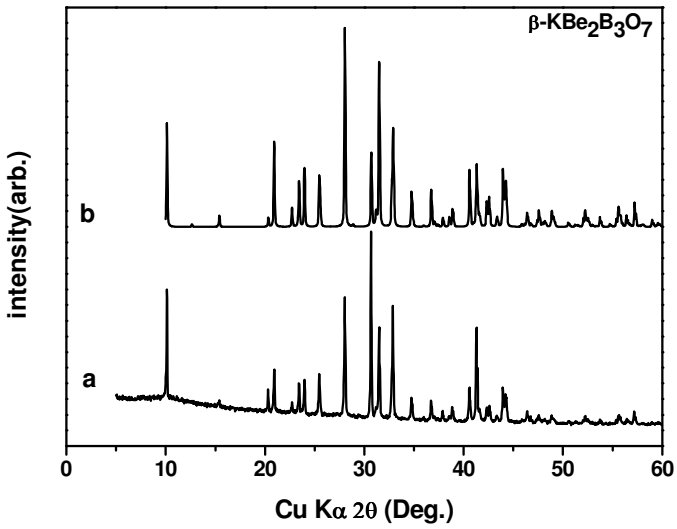
Figure S2. The crystal pictures of $NaBeB_3O_6$ and $ABe_2B_3O_7$ (A = K, Rb)



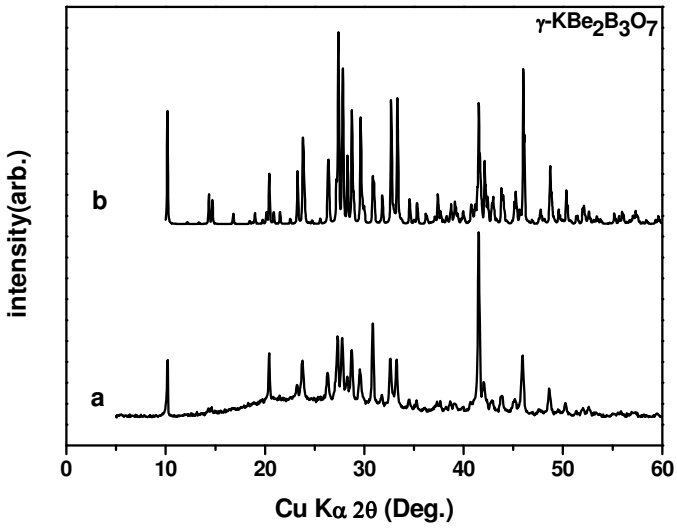
a. X-ray powder diffraction patterns of $NaBeB_3O_6$



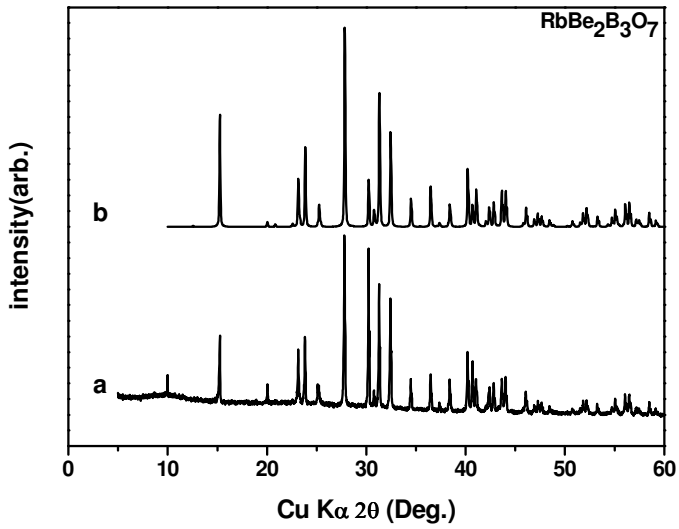
b. X-ray powder diffraction patterns of α-$KBe_2B_3O_7$



c. X-ray powder diffraction patterns of β-$KBe_2B_3O_7$



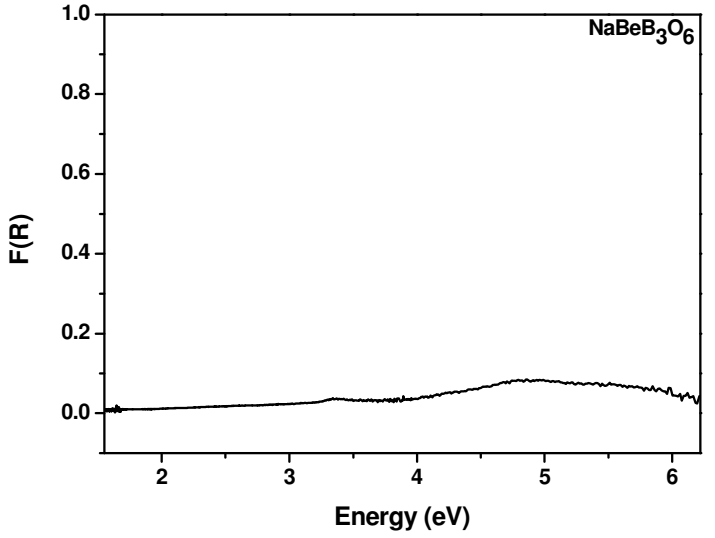
d. X-ray powder diffraction patterns of γ-$KBe_2B_3O_7$



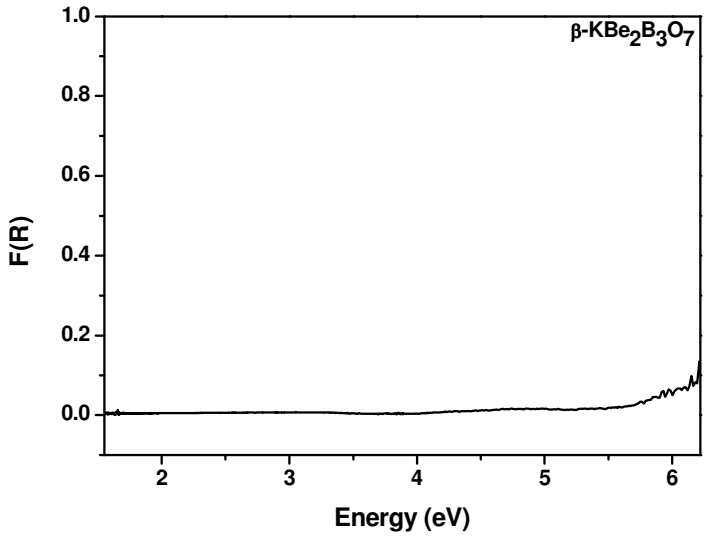
e. X-ray powder diffraction patterns of $RbBe_2B_3O_7$

Figure S3. X-ray powder diffraction patterns of $NaBeB_3O_6$ and $ABe_2B_3O_7$ (A = K, Rb)

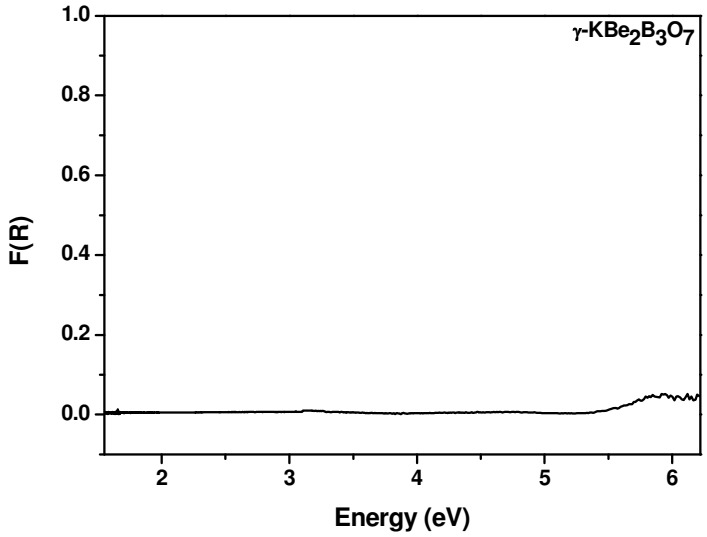
(a) crystal sample and (b) simulation results



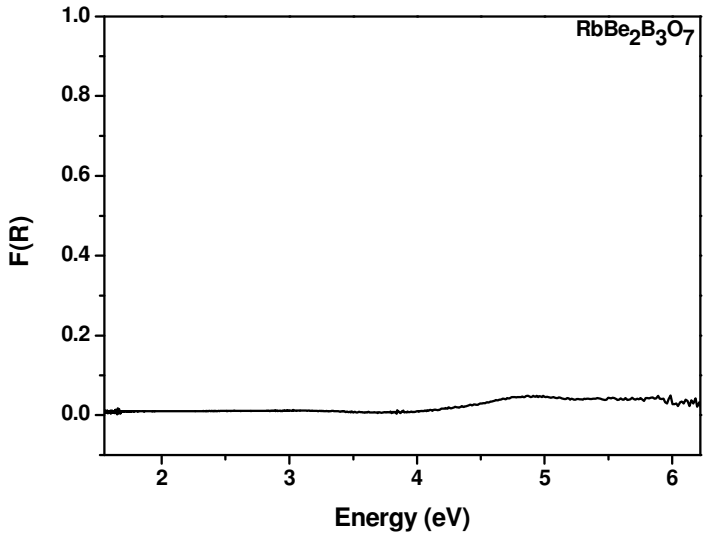
a. Diffuse reflectance absorption curve of the powder sample of $NaBeB_3O_6$



b. Diffuse reflectance absorption curve of the powder sample of β-$KBe_2B_3O_7$



c. Diffuse reflectance absorption curve of the powder sample of γ-$KBe_2B_3O_7$



d. Diffuse reflectance absorption curve of the powder sample of $RbBe_2B_3O_7$

Figure S4. Diffuse reflectance absorption curve of the powder sample of $NaBeB_3O_6$, β-$KBe_2B_3O_7$, γ-$KBe_2B_3O_7$ and $RbBe_2B_3O_7$