crystals

Supplementary Materials: Structure and Optical Properties of $K_{0.67}Rb_{1.33}Al_2B_2O_7$ Crystal

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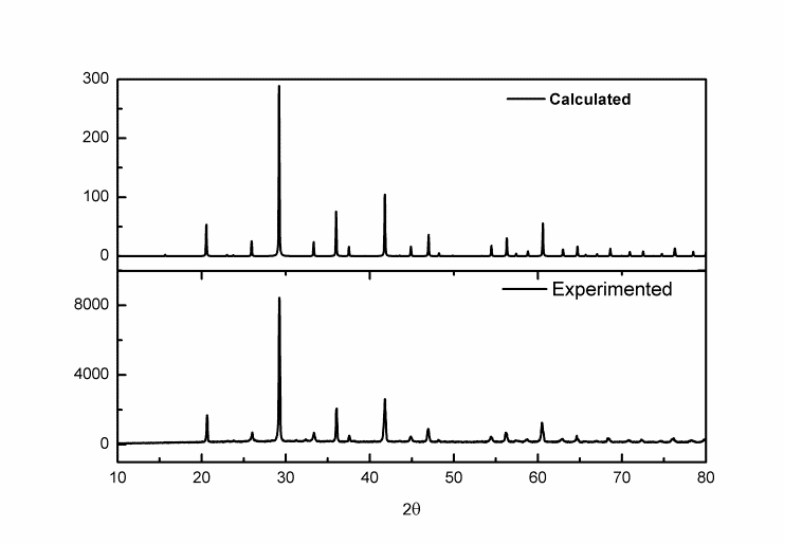

Figure S1. X-ray powder diffraction patterns of KRABO

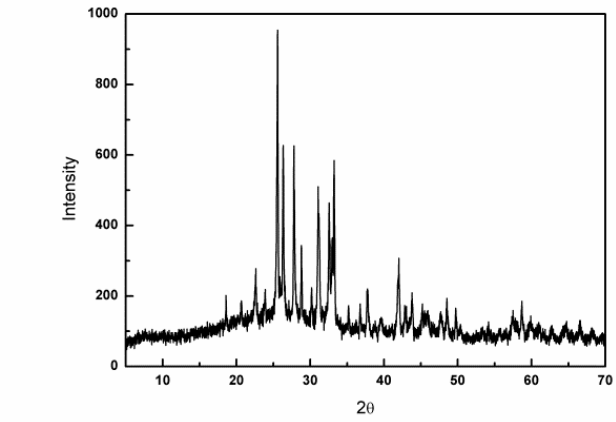

Figure S2. X-ray powder diffraction patterns of KRABO after heated at 1200ºC

Table S1. Crystal data and structure refinement for KRABO

Empirical formula	**$K_{0.67}$ $Rb_{1.33}Al_2B_2O_7$**
Formula weight	327.61
Wavelength(Å)	0.71073
Crystal system	trigonal
Space group	P321
Cell paremeters(Å)	a=b=8.6352(12) c=8.6433(17)
Volume(Å)	558.15(16)

Z	3
Density(g/cm^3)	2.924
F(000)	462
Crystal size(mm^3)	0.109×0.105×0.05
R indices[I＞2σ(I)]	0.0418
R indices(all data)	0.0464

Table S2. Atomic coordinates and equivalent isotropic displacement parameters for KRABO

Atom	x	y	z	U_{eq}(Å^2)
Rb1	0.64258(12)	0	1/2	0.0135(4)
K1	0.64258(12)	0	1/2	0.0135(4)
Rb2	0.69061(13)	0	0	0.0141(5)
K2	0.69061(13)	0	0	0.0141(5)
Al1	1.00000	0	0.3028(3)	0.0054(51)
Al2	2/3	1/3	0.1851(6)	0.0128(15)
Al3	1/3	-1/3	0.2164(6)	0.0145(19)
O1	1.00000	0	1/2	0.021(4)
O2	0.2768(6)	-0.1782(6)	0.2812(6)	0.011(2)
O3	0.9463(6)	0.1581(6)	0.2304(6)	0.0083(19)
O4	0.6072(7)	0.4871	0.2500(8)	0.020(3)
O5	2/3	1/3	-0.0158(14)	0.031(4)
B1	0.6682(15)	0.6624(15)	0.2526(12)	0.010(4)

Table S3. Calculated linear and nonlinear optical properties coefficients

	d_{11}	n_x	n_y	n_z	Δn(1064 nm)
KRABO	0.395	1.55604	1.55604	1.50198	0.054

It is well known that the energy band gaps calculated by standard DFT method are smaller than the measured values, due to the discontinuity of exchange-correlation energy. The scissor operators[1] were adopted to shift all the conduction bands to match the calculated band gaps with the measured values. Based on the scissor-corrected electron band structure, the imaginary part of the dielectric function was calculated according to the electron transition from the valence bands (VB) to conduction band (CB). Consequently, the real part of the dielectric function is obtained by the Kramers-Kronig[2] transform and the refractive index is determined. The SHG coefficients d_{ij} were obtained by the formula developed by our group[3].

References

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2. Palik, E. D., *Handbook of Optical Constants of Solids*. Academic Press: New York, 1985.
3. (a) Lin, J.; Lee, M. H.; Liu, Z. P.; Chen, C. T.; Pickard, C. J., Mechanism for linear and nonlinear optical effects in beta-BaB2O4 crystals. *PhRvB* **1999,** *60* (19), 13380-13389; (b) Lin, Z. S.; Jiang, X. X.; Kang, L.; Gong, P. F.; Luo, S. Y.; Lee, M. H., First-principles materials applications and design of nonlinear optical crystals. *Journal of Physics D-Applied Physics* **2014,** *47* (25), 253001.