Supporting Information

From $BaAlBO_3F_2$ to $BaAlB_3O_6F_2$ and $BaAl_2(B_3O_6)_2F_2$: the Enhancement of Birefringence and Band Gap by Extending the π-Conjugated System Combined with [Al-O/F] Functional Groups

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References

Table S1. Crystal data and structure refinements for $BaAlB_3O_6F_2$ and $BaAl_2(B_3O_6)_2F_2$.

Empirical formula	$BaAlB_3O_6F_2$	$BaAl_2(B_3O_6)_2F_2$
Formula weight	330.75	486.16
Temperature [K]	273(2)	273(2)
Crystal system	monoclinic	trigonal
Space group (number)	$P2_1/c$ (14)	$R\bar{3}c$ (167)
a [Å]	7.1245(6)	7.0654(18)
b [Å]	12.7080(10)	7.0654(18)
c [Å]	7.6246(7)	37.529(13)
α [°]	90	90
β [°]	112.189(3)	90
γ [°]	90	120
Volume [Å^3]	639.19(10)	1622.5(10)
Z	4	6
ρ_{calc} [g cm^{-3}]	3.437	2.958
μ [mm^{-1}]	6.381	3.935
F (000)	600	1356
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2Θ range [°]	6.41 to 55.12	6.51 to 65.56
Index ranges	$-9 \le h \le 9$	$-10 \le h \le 10$
	$-16 \le k \le 15$	$-10 \le k \le 10$
	$-9 \le l \le 9$	$-55 \le l \le 54$
Reflections collected	15684	17663
Independent reflections	1457	644
	R_{int} = 0.0250	R_{int} = 0.0250
	R_{sigma} = 0.0115	R_{sigma} = 0.0115
Completeness	98.9 %	100.0 %
Data / Restraints / Parameters	1457/0/118	644/0/36
Goodness-of-fit on F^2	1.141	1.082
Final R indexes [$I \ge 2\sigma(I)$][a]	R_1 = 0.0110, wR_2 = 0.0277	R_1 = 0.0346, wR_2 = 0.0759
Final R indexes [all data][a]	R_1 = 0.0113, wR_2 = 0.0278	R_1 = 0.0612, wR_2 = 0.0850
Largest peak/hole [eÅ^{-3}]	0.32/-0.45	1.00/-1.52

[a] $R_1 = F_o - F_c/F_o$ and $wR_2 = [w (F_o^2 - F_c^2)^2/wF_o^4]^{1/2}$ for $F_o^2 > 2(F_o^2)$.

Table S2. Atomic coordinates and equivalent isotropic displacement parameters for $BaAlB_3O_6F_2$. U(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*BVS*
Ba1	-0.15914(2)	0.14249(2)	0.87733(2)	0.00965(4)	2.3
Al1	-0.04628(8)	0.09632(4)	0.38295(7)	0.00789(10)	3.1
B1	0.2955(3)	0.23551(16)	0.5266(3)	0.0105(4)	3.0
B2	0.5292(3)	0.39297(15)	0.6556(3)	0.0094(4)	3.0
B3	0.6407(3)	0.56044(16)	0.8284(3)	0.0109(4)	3.0
O1	0.11738(19)	0.21076(10)	0.39411(19)	0.0116(3)	2.1
O2	0.3522(2)	0.34022(10)	0.5523(2)	0.0136(3)	1.9
O3	0.7143(2)	0.35447(10)	0.69269(19)	0.0111(3)	2.0
O4	0.49269(19)	0.49536(10)	0.7083(2)	0.0140(3)	2.1
O5	0.83160(19)	0.52964(10)	0.91797(19)	0.0114(3)	2.2
O6	0.5740(2)	0.66074(10)	0.8511(2)	0.0144(3)	2.1
F1	0.02187(17)	0.03584(9)	0.20052(15)	0.0142(2)	1.1
F2	0.13429(18)	0.16314(9)	0.54769(16)	0.0157(2)	1.0

Table S3. Atomic coordinates and equivalent isotropic displacement parameters for $BaAl_2(B_3O_6)_2F_2$. U(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*BVS*
Ba1	0.666667	0.333333	0.583333	0.02168(17)	1.8
Al1	0.666667	0.333333	0.69801(4)	0.0146(3)	3.1
B1	0.4966(6)	0.6087(6)	0.71292(9)	0.0187(6)	3.0
F1	0.666667	0.333333	0.65367(10)	0.0286(8)	1.0
O1	0.5505(4)	0.8269(4)	0.71260(7)	0.0238(5)	1.9
O2	0.6542(3)	0.5590(3)	0.71370(6)	0.0213(5)	2.0

Table S4. Bond lengths [Å] for $BaAlB_3O_6F_2$.

Atom-Atom	lengths	Atom-Atom	lengths
Ba1–F2	2.5987(12)	Al1–O1	1.8458(14)
Ba1–F1$^{\#1}$	2.6234(11)	Al1–O3$^{\#7}$	1.8806(14)
Ba1–F1$^{\#2}$	2.6780(11)	Al1–O5$^{\#7}$	1.8883(14)
Ba1–O1$^{\#3}$	2.6805(13)	Al1–O5$^{\#8}$	1.8995(14)
Ba1–F2$^{\#3}$	2.7652(12)	Al1–Al1$^{\#1}$	2.9538(10)
Ba1–O6$^{\#4}$	2.8166(13)	B1–O1	1.327(2)
Ba1–O3$^{\#5}$	2.8697(14)	B1–O2	1.383(2)
Ba1–O4$^{\#4}$	2.8979(13)	B1–O6$^{\#8}$	1.408(2)
Ba1–O3$^{\#6}$	3.0155(13)	B2–O3	1.333(2)
Ba1–B3$^{\#4}$	3.355(2)	B2–O2	1.382(2)
Ba1–B1$^{\#3}$	3.377(2)	B2–O4	1.415(2)
Ba1–Al1$^{\#3}$	3.4117(6)	B3–O5	1.329(2)
Al1–F1	1.8088(12)	B3–O4	1.381(2)
Al1–F2	1.8130(13)	B3–O6	1.394(2)

Symmetry transformations used to generate equivalent atoms:
#1:-X, -Y, 1-Z; #2: +X, +Y, 1+Z; #3: +X, 0.5-Y, 0.5+Z; #4: -X, -0.5+Y, 1.5-Z; #5: -1+X, 0.5-Y, 0.5+Z; #6: -1+X, +Y, +Z; #7: -1+X, 0.5-Y, -0.5+Z; #8: 1-X, -0.5+Y, 1.5-Z; #9: +X, 0.5-Y, -0.5+Z; #10: +X, +Y, -1+Z; #11: -X, 0.5+Y, 1.5-Z; #12: 1+X, 0.5-Y, 0.5+Z; #13: 1+X, 0.5-Y, -0.5+Z; #14: 1+X, +Y, +Z; #15: 1-X, 0.5+Y, 1.5-Z;

Table S5. Bond angles [deg] for $BaAlB_3O_6F_2$.

Atom–Atom–Atom	Angle [°]	Atom–Atom–Atom	Angle [°]
F2–Ba1–F1	72.61(3)	F1–Ba1–B3	91.64(4)
F2–Ba1–F1	139.11(3)	F1–Ba1–B3	108.97(4)
F1–Ba1–F1	71.33(4)	O1–Ba1–B3	147.35(4)
F2–Ba1–O1	70.04(4)	F2–Ba1–B3	111.72(4)
F1–Ba1–O1	106.36(4)	O6–Ba1–B3	24.14(4)
F1–Ba1–O1	102.61(4)	O3–Ba1–B3	78.84(4)
F2–Ba1–F2	110.39(2)	O4–Ba1–B3	24.12(4)
F1–Ba1–F2	156.16(4)	O3–Ba1–B3	89.23(4)
F1–Ba1–F2	95.55(3)	F2–Ba1–B1	82.68(5)
O1–Ba1–F2	55.98(4)	F1–Ba1–B1	94.63(4)
F2–Ba1–O6	80.36(4)	F1–Ba1–B1	81.66(4)
F1–Ba1–O6	108.96(4)	O1–Ba1–B1	21.64(4)
F1–Ba1–O6	129.70(4)	F2–Ba1–B1	63.16(4)
O1–Ba1–O6	123.56(4)	O6–Ba1–B1	145.02(4)
F2–Ba1–O6	94.76(4)	O3–Ba1–B1	106.05(4)
F2–Ba1–O3	165.20(4)	O4–Ba1–B1	166.56(4)
F1–Ba1–O3	117.59(3)	O3–Ba1–B1	80.03(4)
F1–Ba1–O3	55.27(3)	B3–Ba1–B1	168.99(5)
O1–Ba1–O3	114.11(4)	F2–Ba1–Al1	79.17(3)
F2–Ba1–O3	65.10(3)	F1–Ba1–Al1	137.48(3)
O6–Ba1–O3	85.90(4)	F1–Ba1–Al1	116.84(3)
F2–Ba1–O4	101.35(4)	O1–Ba1–Al1	32.55(3)
F1–Ba1–O4	74.68(4)	F2–Ba1–Al1	32.01(3)
F1–Ba1–O4	87.12(4)	O6–Ba1–Al1	96.60(3)
O1–Ba1–O4	170.08(4)	O3–Ba1–Al1	97.09(3)
F2–Ba1–O4	125.72(4)	O4–Ba1–Al1	143.12(3)
O6–Ba1–O4	48.25(4)	O3–Ba1–Al1	33.31(3)
O3–Ba1–O4	72.96(4)	B3–Ba1–Al1	120.19(4)
F2–Ba1–O3	64.90(4)	B1–Ba1–Al1	50.03(4)
F1–Ba1–O3	137.51(4)	F1–Al1–F2	174.49(6)
F1–Ba1–O3	146.81(4)	F1–Al1–O1	91.25(6)
O1–Ba1–O3	59.04(4)	F2–Al1–O1	88.67(6)
F2–Ba1–O3	51.40(4)	F1–Al1–O3	88.68(6)
O6–Ba1–O3	65.09(4)	F2–Al1–O3	85.89(6)
O3–Ba1–O3	104.23(3)	O1–Al1–O3	98.44(6)
O4–Ba1–O3	113.33(4)	F1–Al1–O5	91.17(6)
F2–Ba1–B3	90.59(5)	F2–Al1–O5	90.04(6)

Symmetry transformations used to generate equivalent atoms:

#1:-X, -Y, 1-Z; #2: +X, +Y, 1+Z; #3: +X, 0.5-Y, 0.5+Z; #4: -X, -0.5+Y, 1.5-Z; #5: -1+X, 0.5-

Y, 0.5+Z; #6: -1+X, +Y, +Z; #7: -1+X, 0.5-Y, -0.5+Z; #8: 1-X, -0.5+Y, 1.5-Z; #9: +X, 0.5-Y, -0.5+Z; #10: +X, +Y, -1+Z; #11: -X, 0.5+Y, 1.5-Z; #12: 1+X, 0.5-Y, 0.5+Z; #13: 1+X, 0.5-Y, -0.5+Z; #14: 1+X, +Y, +Z; #15: 1-X, 0.5+Y, 1.5-Z;

Table S6. Bond lengths [Å] for $BaAl_2(B_3O_6)_2F_2$.

Atom-Atom	lengths	Atom-Atom	lengths
Ba1–F1#1	2.640(4)	Ba1–O2#3	3.150(2)
Ba1–F1	2.640(4)	Ba1–O2#6	3.150(2)
Ba1–O1#2	3.109(2)	Al1–F1	1.664(4)
Ba1–O1#3	3.109(3)	Al1–O2#8	1.743(2)
Ba1–O1#4	3.109(3)	Al1–O2	1.743(2)
Ba1–O1#5	3.109(3)	Al1–O2#9	1.743(2)
Ba1–O1#6	3.109(3)	B1–O2	1.325(4)
Ba1–O1#7	3.109(2)	B1–O1	1.390(4)
Ba1–O2#2	3.150(2)	B1–O1#10	1.392(4)
Ba1–O2#4	3.150(2)		

Symmetry transformations used to generate equivalent atoms:
#1: -3.66667+X-Y, 1.66667-Y, 1.16667-Z; #2: 0.66667-X+Y, -0.66667+Y, -0.16667+Z; #3: -0.33333+X, 0.33333+X-Y, -0.16667+Z; #4: 1.66667-Y, 1.33333-X, -0.16667+Z; #5: 1.66667-X, 1.33333-Y, 1.33333-Z; #6: 0.66667+X-Y, -0.66667+X, 1.33333-Z; #7: -0.33333+Y, 0.33333-X+Y, 1.33333-Z; #8: 1-X+Y, 1-X, +Z; #9: 1-Y, +X-Y, +Z; #10: -X+Y, 1-X, +Z; #11: 1-Y, 1+X-Y, +Z;

Table S7. Bond angles [deg] for $BaAl_2(B_3O_6)_2F_2$.

Atom–Atom–Atom	Angle [°]	Atom–Atom–Atom	Angle [°]
F1–Ba1–F1	180.0	O1–Ba1–O2	58.03(6)
F1–Ba1–O1	63.16(5)	O1–Ba1–O2	149.32(6)
F1–Ba1–O1	116.83(5)	O1–Ba1–O2	104.79(6)
F1–Ba1–O1	63.17(5)	O2–Ba1–O2	102.67(5)
F1–Ba1–O1	116.83(5)	F1–Ba1–O2	64.37(4)
O1–Ba1–O1	101.21(6)	F1–Ba1–O2	115.63(4)
F1–Ba1–O1	63.17(5)	O1–Ba1–O2	126.55(6)
F1–Ba1–O1	116.83(5)	O1–Ba1–O2	44.03(6)
O1–Ba1–O1	101.21(6)	O1–Ba1–O2	62.47(6)
O1–Ba1–O1	101.21(6)	O1–Ba1–O2	149.32(6)
F1–Ba1–O1	116.84(5)	O1–Ba1–O2	104.79(6)
F1–Ba1–O1	63.16(5)	O1–Ba1–O2	58.03(6)
O1–Ba1–O1	68.88(9)	O2–Ba1–O2	102.67(5)
O1–Ba1–O1	166.53(9)	O2–Ba1–O2	102.67(5)
O1–Ba1–O1	89.95(9)	F1–Ba1–O2	115.63(4)
F1–Ba1–O1	116.84(5)	F1–Ba1–O2	64.37(4)
F1–Ba1–O1	63.16(5)	O1–Ba1–O2	58.03(6)
O1–Ba1–O1	89.95(9)	O1–Ba1–O2	104.79(6)
O1–Ba1–O1	68.88(9)	O1–Ba1–O2	149.32(6)
O1–Ba1–O1	166.53(9)	O1–Ba1–O2	62.46(6)
O1–Ba1–O1	101.20(6)	O1–Ba1–O2	44.03(6)
F1–Ba1–O1	116.84(5)	O1–Ba1–O2	126.54(6)
F1–Ba1–O1	63.16(5)	O2–Ba1–O2	56.12(8)
O1–Ba1–O1	166.53(9)	O2–Ba1–O2	106.07(8)
O1–Ba1–O1	89.95(9)	O2–Ba1–O2	147.34(8)
O1–Ba1–O1	68.88(9)	F1–Al1–O2	109.75(9)
O1–Ba1–O1	101.20(6)	F1–Al1–O2	109.75(9)
O1–Ba1–O1	101.20(6)	O2–Al1–O2	109.19(9)
F1–Ba1–O2	64.37(4)	F1–Al1–O2	109.75(9)
F1–Ba1–O2	115.63(4)	O2–Al1–O2	109.19(9)
O1–Ba1–O2	44.03(6)	O2–Al1–O2	109.19(9)
O1–Ba1–O2	62.47(6)	O2–B1–O1	119.5(3)
O1–Ba1–O2	126.55(6)	O2–B1–O1	122.3(3)
O1–Ba1–O2	104.79(6)	O1–B1–O1	118.2(3)
O1–Ba1–O2	58.03(6)	Al1–F1–Ba1	180.0
O1–Ba1–O2	149.32(6)	B1–O1–B1	121.8(3)
F1–Ba1–O2	64.37(4)	B1–O1–Ba1	95.29(19)
F1–Ba1–O2	115.63(4)	B1–O1–Ba1	134.4(2)

O1–Ba1–O2	62.47(6)	B1–O2–Al1	132.0(2)
O1–Ba1–O2	126.55(6)	B1–O2–Ba1	95.0(2)
O1–Ba1–O2	44.03(6)	Al1–O2–Ba1	133.00(10)

Symmetry transformations used to generate equivalent atoms:
#1: -3.66667+X-Y, 1.66667-Y, 1.16667-Z; #2: 0.66667-X+Y, -0.66667+Y, -0.16667+Z; #3: -0.33333+X, 0.33333+X-Y, -0.16667+Z; #4: 1.66667-Y, 1.33333-X, -0.16667+Z; #5: 1.66667-X, 1.33333-Y, 1.33333-Z; #6: 0.66667+X-Y, -0.66667+X, 1.33333-Z; #7: -0.33333+Y, 0.33333-X+Y, 1.33333-Z; #8: 1-X+Y, 1-X, +Z; #9: 1-Y, +X-Y, +Z; #10: -X+Y, 1-X, +Z; #11: 1-Y, 1+X-Y, +Z;

Table S8. Comparison of bandgap and birefringence for the known F-containing aluminoborates and the arrangement of the [Al-O/F] groups.

	Compound	Band gap / eV	Cut-off edge / nm	birefringence	[Al-O/F]
Aluminoborate fluorides	$K_3Ba_3Li_2Al_4B_6O_{20}F$[1]	＞6.2	＜190	0.063	[AlO_4]
	$K_3Sr_3Li_2Al_4B_6O_{20}F$[2]	＞6.2	190	0.062	[AlO_4]
	$Rb_3Ba_3Li_2Al_4B_6O_{20}F$[3]	＞6.2	198	0.061	[AlO_4]
Fluoroaluminoborates	$BaAlBO_3F_2$[4]	＞6.2	165	0.0418	[AlO_3F_2]
	$Rb_3Al_3B_3O_{10}F$[5]	6.58*	＜200	/	[AlO_3F]
	$CsAlB_3O_6F$[6]	7.49*	＜190	0.091	[AlO_3F]
	$RbAlB_3O_6F$[7]	7.15*	＜190	0.0946	[AlO_3F]
	$Cs_{0.5}Rb_{0.5}AlB_3O_6F$[7]	＞6.2	＜200	/	[AlO_3F]
	$Li_{0.5}Na_{0.5}AlB_2O_4F_2$[8]	7.55*	＜200	0.108	[AlO_3F_3]
	$SrAlB_3O_6F_2$[9]	7.65*	＜200	0.075	[AlO_4F_2]
	$Sr_2Al_{2.18}B_{5.82}O_{13}F_2$[10]	7.28*	＜200	0.058	[AlO_4F_2]
	$SnAl_2(BO_3)_2F_2$[11]	4.08	240	0.024	[AlO_4F_2]
	$Al_8(BO_3)_4(B_2O_5)F_8$[12]	7.32*	＜200	/	[AlO_4F_2]
	$Pb_2Al_2B_3O_8F_3$[13]	5.26	213	0.0458	[AlO_4F_2]
	$Pb_6AlB_2O_7F_7$[14]	3.63	＜300	/	[AlF_6]
	$Al_6B_5O_{15}F_3$[15]	/	/	/	[AlO_5F]
	$BaAlB_3O_6F_2$（this work）	**7.53***	＜200	**0.087**	[AlO_4F_2]
	$BaAl_2(B_3O_6)_2F_2$（this work）	**7.87***	＜200	**0.105**	[AlO_3F]

* DFT calculated results

Figure S1. Different arrangement of [Al-O/F] groups in (a) $BaAlBO_3F_2$, (b) $BaAlB_3O_6F_2$, and (c) $BaAl_2(B_3O_6)_2F_2$.

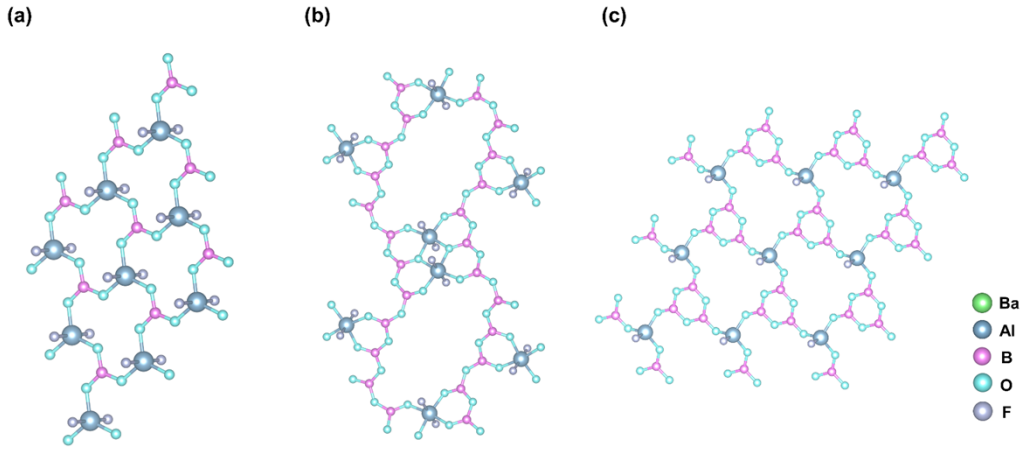


Figure S2. The experimental and calculated sample XRD patterns of (a) $BaAlB_3O_6F_2$ and (b) $BaAl_2(B_3O_6)_2F_2$.

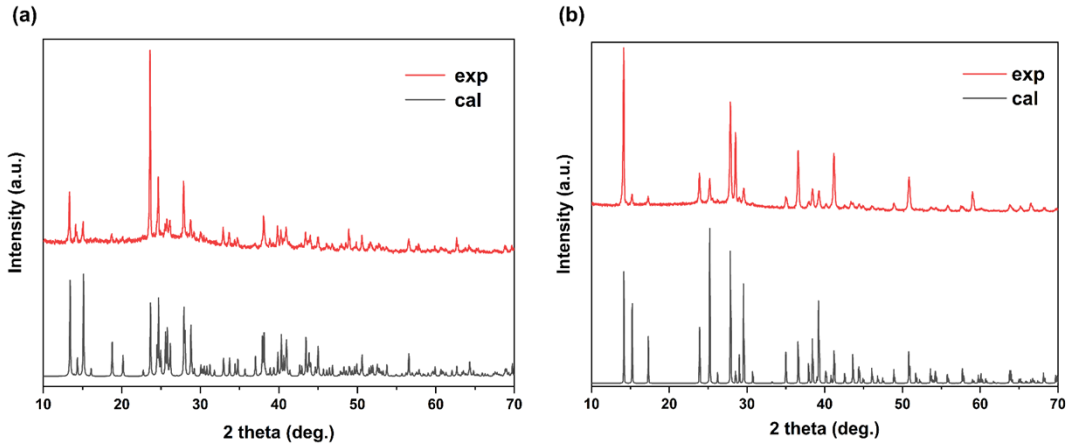


Figure S3. TG/DSC curves of (a) $BaAlB_3O_6F_2$ and (b) $BaAl_2(B_3O_6)_2F_2$.

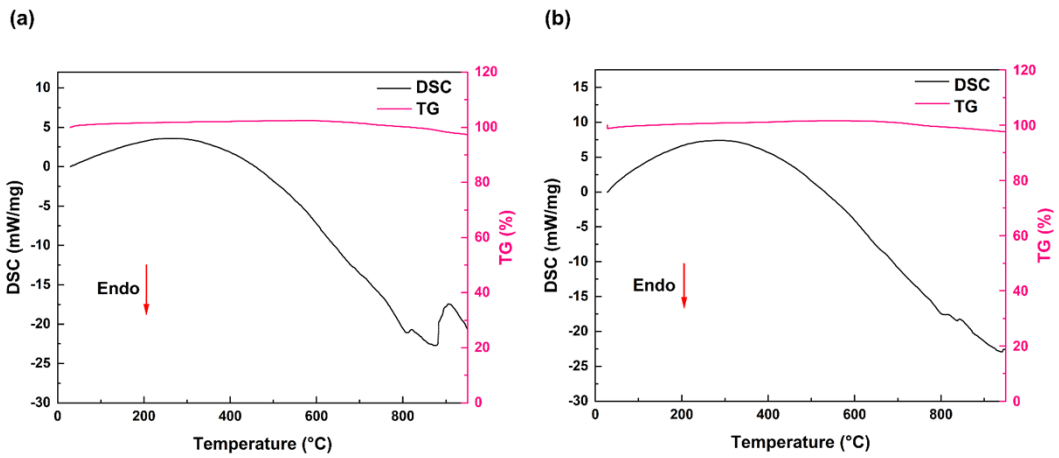


Figure S4. IR Spectra of (a) $BaAlB_3O_6F_2$ and (b) $BaAl_2(B_3O_6)_2F_2$.

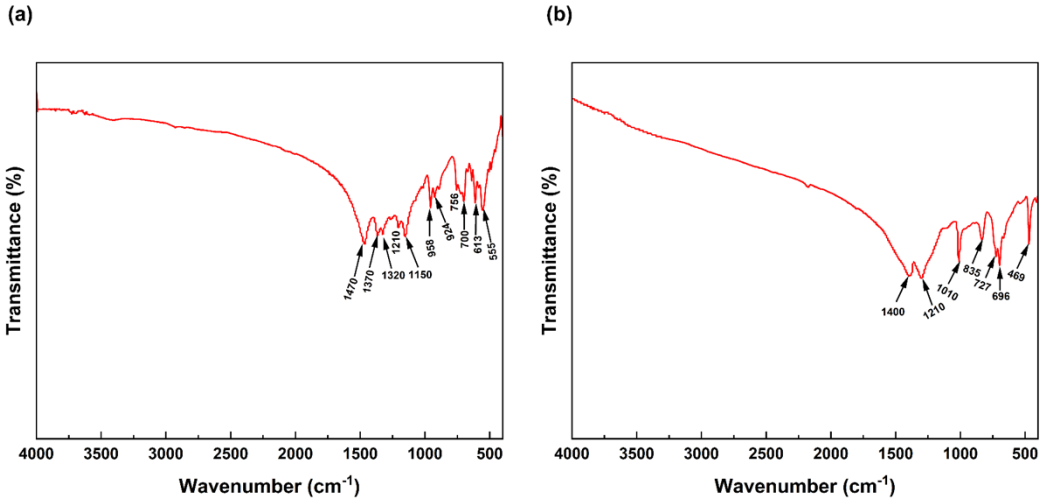


Figure S5. The measurement of thickness of (a) $BaAlB_3O_6F_2$ and (b) $BaAl_2(B_3O_6)_2F_2$.

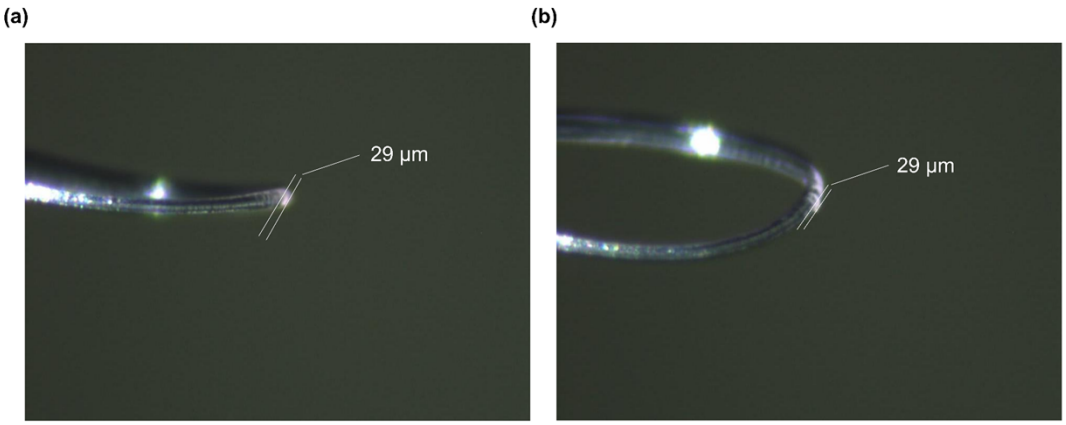
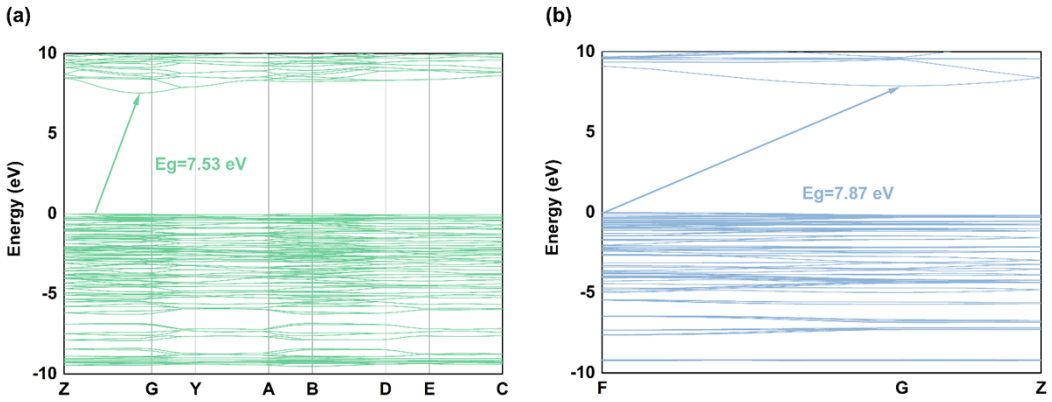


Figure S6. The calculated band gaps (HSE06) of (a) $BaAlB_3O_6F_2$ and (b) $BaAl_2(B_3O_6)_2F_2$.



References

1. B.Q. Zhao, B.X. Li, S.G. Zhao, X.T. Liu, Z.Y. Wu, Y.G. Shen, X.F. Li, Q.R. Ding, C.M. Ji and J.H. Luo, Physical properties of a promising nonlinear optical crystal $K_3Ba_3Li_2Al_4B_6O_{20}F$, *Cryst. Growth Des.,* 2018, ***18***, 7368-7372.
2. Y. Yang, S.Z. Huang and S.L. Pan, $K_3Sr_3Li_2Al_4B_6O_{20}F$: a competitive nonlinear optical crystal for generation of a 266 nm laser, *J. Mater. Chem. C.,* 2022, ***10***, 11232-11238.
3. J.K. Wang, H.P. Wu, Z.G. Hu, J.Y. Wang, Y.C. Wu and H.W. Yu, A promising ultraviolet nonlinear optical crystal: $Rb_3Ba_3Li_2Al_4B_6O_{20}F$—crystal growth, physical properties, and 266 nm laser generation, *J. Mater. Chem. C.,* 2023, ***11***, 1320-1328.
4. Z.G. Hu, M. Yoshimura, K. Muramatsu, Y. Mori and T. Sasaki, A new nonlinear optical crystal-$BaAlBO_3F_2$(BABF), *Jpn. J. Appl. Phys.,* 2002, ***41***, L1131-L1133.
5. S.G. Zhao, P.F. Gong, S.Y. Luo, S.J. Liu, L.N. Li, M.A. Asghar, T.K. Asghar, M.C. Hong, Z.S. Lin and J.H. Luo, Beryllium-free $Rb_3Al_3B_3O_{10}F$ with reinforced interlayer bonding as a deep-ultraviolet nonlinear optical crystal, *J. Am. Chem. Soc.,* 2015, ***137***, 2207-2210.
6. H.K. Liu, Y. Wang, B.B. Zhang, Z.H. Yang and S.L. Pan, $CsAlB_3O_6F$: a beryllium-free deep-ultraviolet nonlinear optical material with enhanced thermal stability, *Chem. Sci.,* 2020, ***11***, 694-698.
7. H.K. Liu, B.B. Zhang, L. Li and Y. Wang, Exploring deep-UV nonlinear optical materials with enhanced second harmonic generation response and birefringence in fluoroaluminoborate crystals, *ACS Appl. Mater. Interfaces.,* 2021, ***13***, 30853-30860.
8. Z.T. Yan, D.D. Chu, M. Zhang, Z.H. Yang and S.L. Pan, $Li_{0.5}Na_{0.5}AlB_2O_4F_2$: fluoroaluminoborate with aligned $^{1\infty}[BO_2]$ chain induced by unprecedented $[AlO_3F_3]^{6-}$ species features enhanced birefringence, *Adv. Opt. Mater.,* 2022, ***11***, 2202353.
9. S. Bai, X.D. Zhang, B.B. Zhang, L. Li and Y. Wang, $SrAlB_3O_6F_2$: A fluoroaluminoborate with $[Al_2B_6O_{14}F_4]$ units and large birefringence, *Inorg. Chem.,* 2021, ***60***, 10006-10011.
10. J.H. Jiao, A. Tudi, Z.T. Yan and M. Zhang, Structural motif cosubstitution strategy for designing fluoroaluminoborate with the $Sr_2Be_2B_2O_7$-type double-layered structure, *Inorg. Chem.,* 2023, ***62***, 4399-4404.
11. Y. Wang, J. Han, J.B. Huang, Z.H. Yang, S.Z. Huang and S.L. Pan, From $BaAl_2(BO_3)_2O$ to $SnAl_2(BO_3)_2F_2$: structure transformation based on ion regulation, *New J. Chem.,* 2020, ***44***, 9852-9857.
12. Y. Wang, J. Han, J.B. Huang, Z.H. Yang and S.L. Pan, $Al_8(BO_3)_4(B_2O_5)F_8$: A F-containing aluminum borate featuring two types of isolated B–O groups, *Inorg. Chem.,* 2019, ***59***, 810-817.
13. B. Jiang, S. Shu, Z.H. Yang, F.F. Zhang, M. Zhang and S.L. Pan, $Pb_2Al_2B_3O_8F_3$: structure and properties of a new fluoroaluminoborate with non-traditional chain-like B_3O_8 groups, *Dalton Trans.,* 2022, ***51***, 3964-3969.
14. L.Y. Dong, S.L. Pan, Z.H. Yang, W.W. Zhao, X.Y. Dong, Y. Wang and Y.N. Huang, Synthesis, crystal structure, and properties of a new lead aluminum fluoride borate,$Pb_6AlB_2O_7F_7$, *Z. Anorg. Allg. Chem.,* 2012, ***638***, 2280-2285.
15. E.V. Sokolova, Y.K. Egorov Tismenko, S.V. Kargal'tsev, V.A. Klyakhin and V.S. Urusov, Refinement of the crystalline structure of synthetic fluorous jeremejevite $Al_6[BO_3]_5F_3$, *Geol. Geofiz.,* 1987, ***42***, 82-84.