Crystal growth, structure and optical properties of a new acentric crystal $La_2Al_{4.68}B_8O_{22}$ with short UV absorption edge

Tittle: **Crystal growth, structure and optical properties of a new acentric crystal $La_2Al_{4.68}B_8O_{22}$ with short UV absorption edge**

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Supporting information

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Table S1 Crystal data and structure refinements for $La_2Al_{4.68}B_8O_{22}$

	$La_2Al_{4.68}B_8O_{22}$
Fw	842.57
T(K)	153.1500
a(Å)	4.6149(7)
b(Å)	4.6149(7)
c(Å)	18.720(4)
α(°)	90
β (°)	90
γ (°)	120
Space group	*P-62m*
V(Å^3)	345.27(15)
Z	1
ρ_c(g/cm^3)	4.052
μ(cm^{-1})	6.557
$R(F)^a$	0.0379(403)
$R_W(F_o^2)^b$	0.1322(475)

Table S2 Selected interatomic distances (Å) for $La_2Al_{4.68}B_8O_{22}$

La1—O3	2.464(3)	Al1—Al1	2.471(3)
La1—O3	2.464(3)	Al1—Al1	2.471(3)
La1—O3	2.464(3)	O1—Al1	1.799(5)
La1—O3	2.464(3)	O1—Al1	1.799(5)
La1—O3	2.464(3)	O2—B1	1.442(9)
La1—O3	2.464(3)	O2—Al1	1.844(3)
La2—O4	2.493(3)	O2—Al1	1.844(3)
La2—O4	2.493(3)	O3—B1	1.490(3)
La2—O4	2.493(3)	O3—B1	1.490(3)
La2—O4	2.493(3)	O3—La1	2.464(3)
La2—O4	2.493(3)	O4—B2	1.491(3)
La2—O4	2.493(3)	O4—B2	1.491(3)
Al1—O1	1.799(5)	O5—B2	1.410(9)
Al1—O2	1.844(3)	O5—Al1	1.851(3)
Al1—O2	1.844(3)	O5—Al1	1.851(3)
Al1—O5	1.851(3)	B1—O3	1.490(3)
Al1—O5	1.851(3)	B1—O3	1.490(3)
Al1—Al1	2.471(3)	B2—O4	1.491(3)
Al1—Al1	2.471(3)	B2—O4	1.491(3)

Table S3. Positional coordinates for $La_2Al_{4.68}B_8O_{22}$.

Atom	Wyckoff	x/a	y/b	z/c
La1	1a	0	0	0
La2	1b	0	0	1/2
Al1	6i	0.3896(11)	0.3896(11)	0.24972(6)
O1	2e	0	0	0.2525(5)
O2	4h	2/3	1/3	0.1873(3)
O3	6i	0.5760(8)	0	0.08003(15)
O4	6i	0.4294(7)	0	0.41920(14)
O5	4h	2/3	1/3	0.3127(2)
B1	4h	2/3	1/3	0.1103(4)
B2	4h	2/3	1/3	0.3880(4)

Table S4 Measured and calculated refractive indexes of $La_2Al_{4.68}B_8O_{22}$

λ (nm)	n_o		n_e		Δn
	Exp	Cal	Exp	Cal	
253.7	1.81701	1.81698	1.79529	1.79524	0.02172
363	1.75810	1.75851	1.73947	1.73997	0.01863
404.7	1.74919	1.74902	1.73098	1.73092	0.01821
435.8	1.74391	1.74379	1.72607	1.72592	0.01784
480	1.73820	1.73811	1.72079	1.72050	0.01741
546.1	1.73218	1.73208	1.71488	1.71475	0.0173
587.5	1.72938	1.72927	1.71218	1.71208	0.0172
643.8	1.72629	1.72623	1.70926	1.70919	0.01703
706.5	1.72352	1.72355	1.70678	1.70667	0.01674
852.1	1.71888	1.71900	1.70267	1.70246	0.01621
1014	1.71511	1.71529	1.69839	1.69911	0.01672
2325	1.68862	1.68859	1.67689	1.67682	0.01173

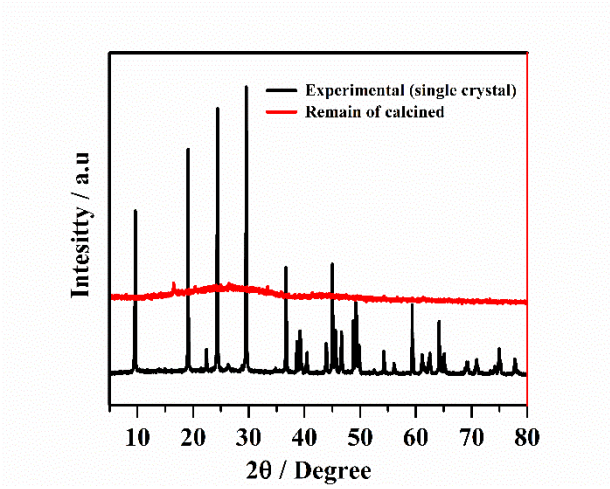

Fig. S1. Comparison of powder X-ray diffraction patterns of LaAB and calcined melt.

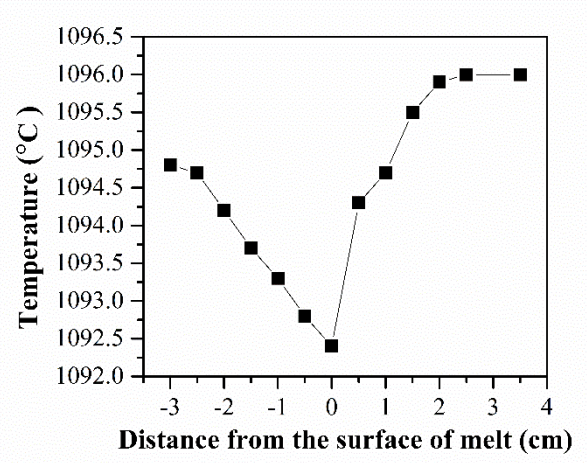

Fig.S2 The temperature field in the axis direction.

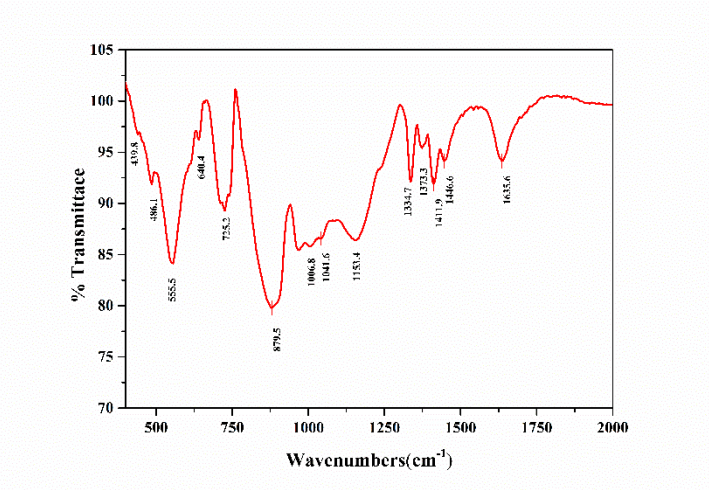

Fig. S3 IR spectrum of LaAB

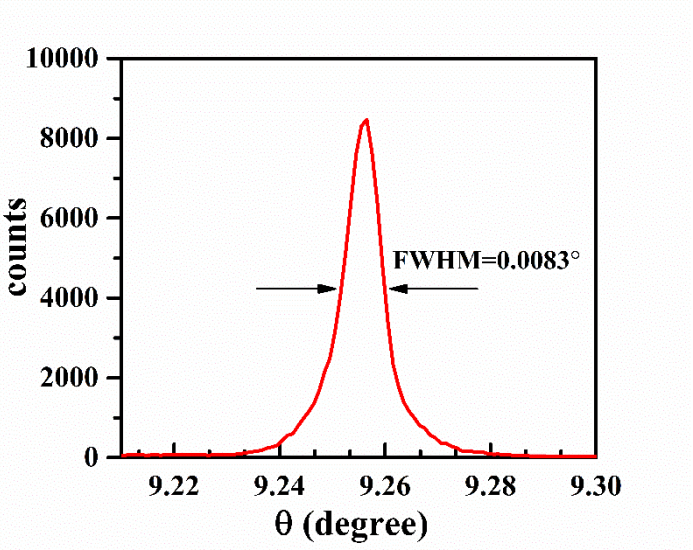

Fig .S4 Rocking curve of the (001) face of the as-grown crystal.