Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Supplementary Information

$LaBeB_3O_7$: A New Phase-matchable Nonlinear Optical Crystal Exclusively Containing the Tetrahedral XO_4 (X = B and Be) Anionic Groups

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Tab. S1. Atomic coordinates and isotropic displacement coefficients.

atom	x	y	z	Wyckoff	U(eq)(Å^2)	occupancy
La(1)	0.5	0.2147(1)	0.2516	2a	0.005(1)	1
B(1)	0.3793(5)	0.682(1)	-0.215(2)	4b	0.004(1)	1
B(2)	0.2502(4)	0.183(1)	-0.228(3)	4b	0.003(1)	0.5
Be(1)	0.2502(4)	0.183(1)	-0.228(3)	4b	0.003(1)	0.5
O(1)	0.2744(4)	0.8571(9)	-0.3671(9)	4b	0.006(1)	1
O(2)	0.3687(3)	0.3629(9)	-0.288(1)	4b	0.004(1)	1
O(3)	0.3713(5)	0.7208(8)	0.124(1)	4b	0.006(1)	1
O(4)	0.5	0.805(1)	-0.325(1)	2a	0.004(1)	1

Tab. S2. Selected Bond Distances (Å) and Angles (°) for $LaBeB_3O_7$ [a]

$LaBeB_3O_7$			
Band distance (Å)			
La(1)-O(4)$^{\#3}$	2.573(5)	(B1)-O(1)	1.511(7)
La(1)-O(2)$^{\#1, \#2}$	2.517(5)*2	(B1)-O(2)	1.456(6)
La(1)-O(3)$^{\#4, \#5}$	2.647(4)*2	(B1)-O(3)	1.47(1)
La(1)-O(3)$^{\#0, \#6}$	2.692(4)*2	(B1)-(O4)	1.477(6)
La(1)-O(2)$^{\#0, \#6}$	2.784(4)*2	$(B(1)\text{-}O)_{average}$	1.478
La(1)-O(1)$^{\#7, \#8}$	2.989(4)*2	B(2)-O(1)$^{\#4}$	1.587(7)
La(1)-O(4)$^{\#10}$	3.077(1)	B(2)-O(1)$^{\#7}$	1.59(1)
La(1)-O(4)$^{\#2}$	3.191(8)	B(2)-O(2)	1.518(6)
La(1)-O(1)$^{\#3, \#11}$	3.317(5)*2	B(2)-O(3)$^{\#7}$	1.507(8)
La(1)-O(4)	3.191(8)	$(B(2)\text{-}O)_{average}$	1.55
$(La(1)\text{-}O)_{average}$	2.897		
Selected bond angle (°)			
O(1)-B(1)-O(2)	110.7(4)	O(1)$^{\#4}$-B(2)-O(1)$^{\#7}$	107.0(4)
O(1)-B(1)-O(3)	109.0(5)	O(1)$^{\#4}$-B(2)-O(2)	106.4(4)
O(1)-B(1)-O(4)	108.5(4)	O(1)$^{\#4}$-B(2)-O(3)$^{\#9}$	103.9(5)
O(2)-B(1)-O(3)	108.6(4)	O(1)$^{\#7}$-B(2)-O(2)	111.0(6)
O(2)-B(1)-O(4)	111.1(4)	O(1)$^{\#7}$-B(2)-O(3)$^{\#9}$	107.7(5)
O(4)-B(1)-O(4)	109.0(5)	O(2)-B(2)-O(3)$^{\#9}$	119.8(5)
$(O\text{-}B(1)\text{-}O)_{average}$	109.5	$(O\text{-}B(2)\text{-}O)_{average}$	109.3

[a]symmetry operations: （#0） x, y, z; (#1) 1-x, y, 1+z; (#2) x, y, 1+z; (#3) x, -1+y, 1+z; (#4) x, -1+y, z; (#5) 1-x, -1+y, z; (#6)1-x, y, z; (#7) 0.5-x, 1-y, 0.5+z; (#8) 0.5+x, 1-y, 0.5+z; (#9) 0.5-x, 1-y,-0.5+z.; (#10) x,-1+y,z; (#11) 1-x, -1+y, 1+z.

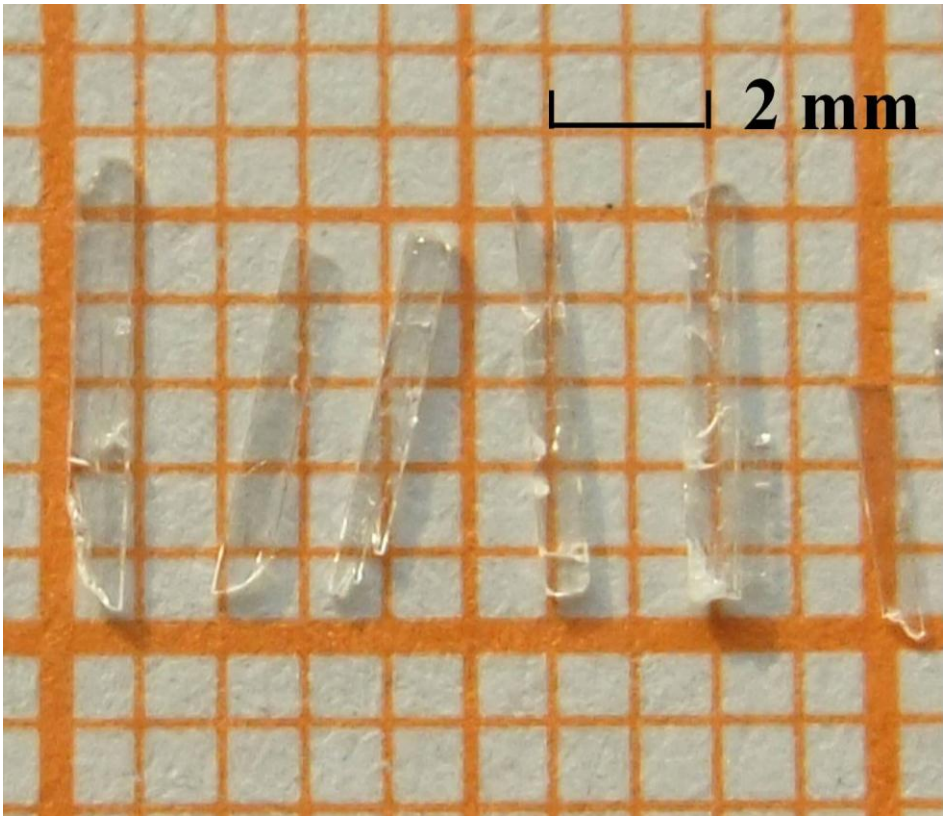

Fig. S1. As-grown $LaBeB_3O_7$ crystals.

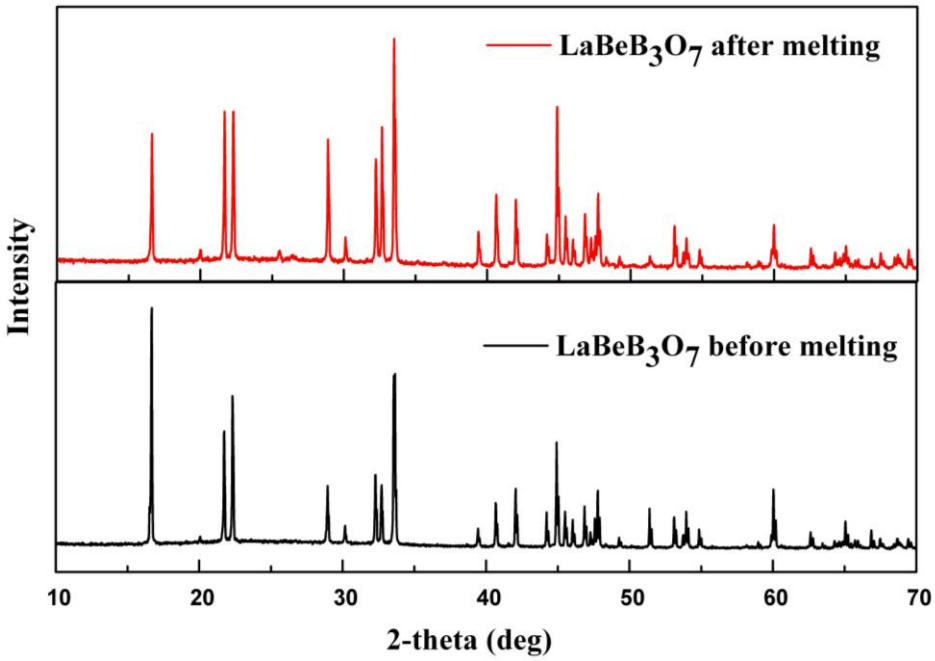

Fig. S2. XRD patterns of the $LaBeB_3O_7$ samples before and after melting, respectively. The black curve is the pattern of $LaBeB_3O_7$ before melting and the red one is the pattern of samples after melting.