

$\text{Li}_3\text{Na}_7\text{B}_4\text{P}_6\text{O}_{26}$: A New Ultraviolet Transparent Congruently-Melting Non-linear Optical Crystal

Sujuan Yu,¹ Jiangtao Fan,¹ Zhanggui Hu, *¹ and Yicheng Wu¹

1. Tianjin Key Laboratory of Functional Crystal Materials, Institute of Functional
Crystal, Tianjin University of Technology, Tianjin 300384, China.

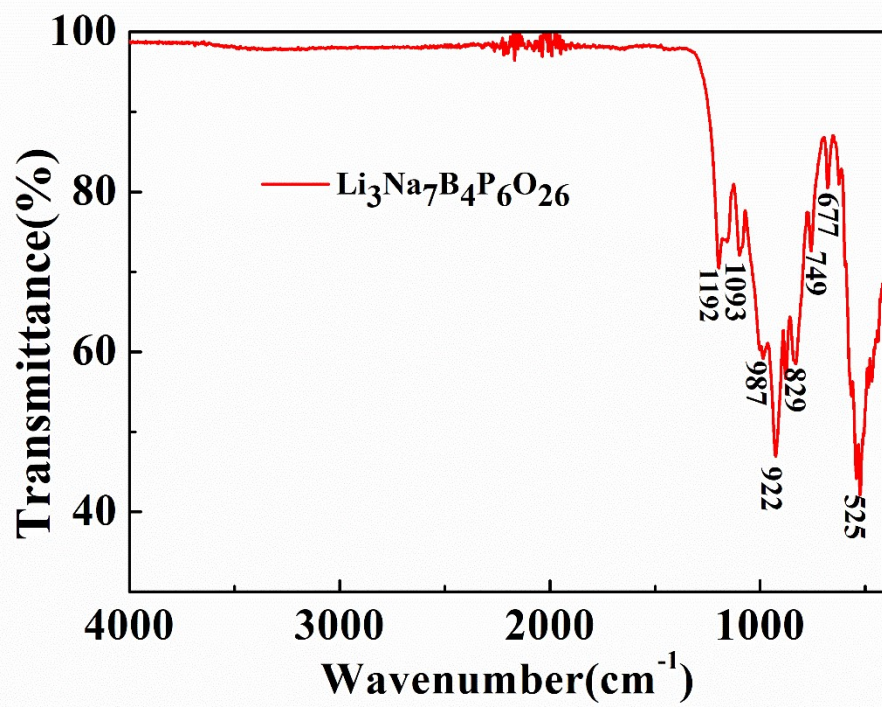


Figure S1 IR spectrum of LNBPO

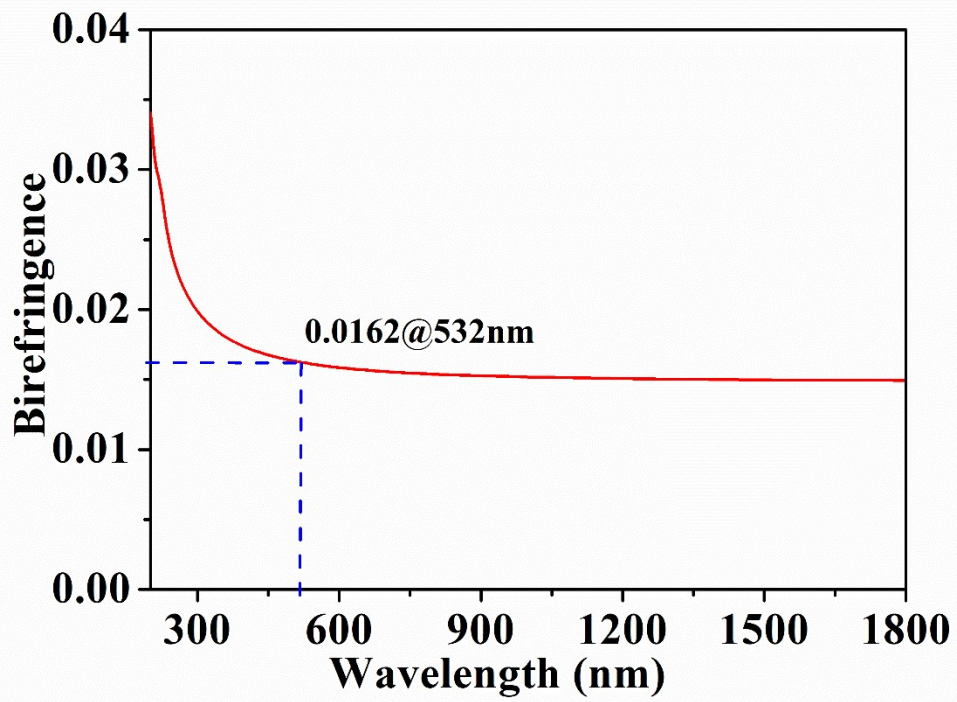


Figure S2 Birefringence curve of LNBPO

Table S1. Crystal data and structure refinements of LNBPO

Empirical formula	$\text{Li}_3\text{Na}_7\text{B}_4\text{P}_6\text{O}_{26}$
Formula weight	826.81
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$Pca2_1$
Unit cell dimensions	$a = 6.6568(6)$ Å $b = 13.6358(12)$ Å $c = 11.3226(12)$ Å
Volume	$1027.76(17)$ Å ³
Z	2
Density (calculated)	2.672 Mg/m ³
Absorption coefficient	0.808 mm ⁻¹
F(000)	808
Crystal size	$0.18 \times 0.16 \times 0.14$ mm ³
Theta range for data collection	2.988 to 27.505° .
Index ranges	$-6 \leq h \leq 7$, $-16 \leq k \leq 14$, $-13 \leq l \leq 13$
Reflections collected	4692
Independent reflections	1732 [R(int) = 0.0588]
Completeness to theta	99.9 %
Refinement method	Full-matrix least-squares on F ²
Goodness-of-fit on F ²	1.067
Final R indices [I > 2σ(I)]	R1 = 0.0500, wR2 = 0.0972
R indices (all data)	R1 = 0.0773, wR2 = 0.1072
Largest diff. peak and hole	0.447 and -0.478 e.Å ⁻³

Table S2. Atoms coordinates and equivalent isotropic displacement parameters for LNBPO

Atoms	x	y	z	U(eq)	BVS
P(1)	2690(4)	7494(2)	5600(3)	14(1)	5.13
Na(1)	8404(15)	7508(7)	6694(9)	30(3)	1.11
Li(2)	2270(30)	8790(11)	8010(20)	18(4)	0.94
P(2)	7599(4)	6021(2)	3349(3)	16(1)	5.07
P(3)	7638(4)	9189(2)	3213(3)	15(1)	5.03
Na(2)	2281(7)	6136(3)	8018(5)	25(1)	1.05
Na(3)	10395(6)	4944(3)	5731(5)	30(1)	0.94
Na(4)	10261(7)	10039(5)	5633(6)	53(2)	0.94
O(1)	8300(11)	7663(5)	4840(7)	13(2)	2.32
O(2)	9587(9)	8522(5)	3155(8)	17(2)	2.05
O(3)	11855(10)	7615(5)	4314(7)	14(2)	2.14
O(4)	9417(9)	6759(5)	3137(8)	15(2)	2.06
O(5)	4943(9)	7775(5)	5435(7)	19(2)	2.11
O(6)	7842(11)	9976(5)	4135(7)	20(2)	1.96
O(7)	5924(11)	8438(5)	3547(7)	19(2)	2.21
O(8)	8085(12)	5283(5)	4268(8)	23(2)	2.04
O(9)	5834(11)	6710(5)	3779(7)	21(2)	2.12
O(10)	7015(10)	5590(5)	2184(8)	23(2)	1.95
O(11)	1765(11)	8243(6)	6417(8)	35(2)	1.98
O(12)	2445(12)	6458(5)	5994(8)	39(2)	1.89
O(13)	7218(11)	9566(6)	2002(8)	28(2)	2.11
B(1)	6277(19)	7636(9)	4435(13)	21(3)	3.05
B(2)	9720(20)	7638(10)	3924(12)	19(3)	3.02
Li(1A)	8540(50)	7940(40)	6630(20)	30(3)	0.59

Symmetry transformations used to generate equivalent atoms:

#1 $x-1,y,z$ #2 $x+1,y,z$ #3 $-x+3/2,y,z+1/2$ #4 $-x+1,-y+2,z+1/2$

#5 $-x+1/2,y,z+1/2$ #6 $-x+1,-y+1,z-1/2$ #7 $-x+1/2,y,z-1/2$

#8 $x-1/2,-y+1,z$ #9 $-x+3/2,y,z-1/2$ #10 $x-1/2,-y+2,z$

#11 $-x+2,-y+2,z-1/2$ #12 $-x+1,-y+1,z+1/2$ #13 $x+1/2,-y+1,z$

#14 $-x+2,-y+1,z+1/2$ #15 $-x+2,-y+2,z+1/2$ #16 $x+1/2,-y+2,z$

#17 $-x+1,-y+2,z-1/2$ #18 $-x+2,-y+1,z-1/2$

Table S3 Selected distances (Å) and angles (deg) for LNBPO

P(1)-O(3)#1	1.567(9)	O(5)-P(1)-O(3)#1	101.7(5)
P(1)-O(5)	1.560(7)	O(11)-P(1)-O(3)#1	110.7(5)
P(1)-O(11)	1.510(9)	O(11)-P(1)-O(5)	107.4(4)
P(1)-O(12)	1.490(8)	O(12)-P(1)-O(3)#1	109.8(5)
Na(1)-O(1)	2.066(11)	O(12)-P(1)-O(5)	112.0(4)
Na(1)-O(1)	2.110(11)	O(12)-P(1)-O(11)	114.5(6)
Na(1)-O(2)#2	2.935(13)	O(1)-Na(1)-O(2)#2	119.4(5)
Na(1)-O(4)#2	2.691(13)	O(1)-Na(1)-O(4)#2	128.2(5)
Na(1)-O(5)	2.733(12)	O(1)-Na(1)-O(5)	56.0(4)
Na(1)-O(7)#2	2.492(13)	O(1)-Na(1)-O(7)#2	142.4(5)
Na(1)-O(9)#2	2.649(13)	O(1)-Na(1)-O(9)#2	159.0(6)
Na(1)-O(10)#2	2.689(12)	O(1)-Na(1)-O(10)#2	107.4(5)
Na(1)-O(11)#3	2.472(13)	O(1)-Na(1)-O(11)#3	82.2(5)
Li(2)-O(2)#2	2.129(19)	O(1)-Na(1)-O(13)#2	91.1(4)
Li(2)-O(3)#2	2.26(2)	O(4)#2-Na(1)-O(2)#2	50.4(3)
Li(2)-O(6)#4	2.11(2)	O(4)#2-Na(1)-O(5)	77.2(3)
Li(2)-O(7)#5	2.27(2)	O(4)#2-Na(1)-O(13)#2	101.4(4)
Li(2)-O(11)	1.98(2)	O(5)-Na(1)-O(2)#2	70.1(3)
Li(2)-O(13)#4	2.536(19)	O(5)-Na(1)-O(13)#2	79.1(3)
P(2)-O(4)	1.593(7)	O(7)#2-Na(1)-O(2)#2	53.7(3)
P(2)-O(8)	1.483(8)	O(7)#2-Na(1)-O(4)#2	78.9(4)
P(2)-O(9)	1.582(8)	O(7)#2-Na(1)-O(5)	121.5(5)
P(2)-O(10)	1.496(9)	O(7)#2-Na(1)-O(9)#2	54.8(3)
P(3)-O(2)	1.586(7)	O(7)#2-Na(1)-O(10)#2	109.8(4)
P(3)-O(6)	1.503(8)	O(7)#2-Na(1)-O(13)#2	54.8(3)
P(3)-O(7)	1.579(8)	O(9)#2-Na(1)-O(2)#2	79.7(4)
P(3)-O(13)	1.491(9)	O(9)#2-Na(1)-O(4)#2	55.7(3)
Na(2)-O(3)#2	2.560(8)	O(9)#2-Na(1)-O(5)	132.9(5)
Na(2)-O(4)#2	2.361(7)	O(9)#2-Na(1)-O(10)#2	55.7(3)
Na(2)-O(8)#13	2.410(9)	O(9)#2-Na(1)-O(13)#2	108.8(4)
Na(2)-O(9)#5	2.378(8)	O(10)#2-Na(1)-O(2)#2	105.8(4)
Na(2)-O(10)#13	2.579(8)	O(10)#2-Na(1)-O(4)#2	55.5(3)
Na(2)-O(12)	2.337(10)	O(10)#2-Na(1)-O(5)	98.6(4)
Na(3)-O(8)#14	2.459(10)	O(10)#2-Na(1)-O(13)#2	156.2(5)
Na(3)-O(8)	2.307(9)	O(11)#3-Na(1)-O(2)#2	119.6(4)
Na(3)-O(10)#15	2.492(9)	O(11)#3-Na(1)-O(4)#2	149.6(5)
Na(3)-O(10)#2	2.460(9)	O(11)#3-Na(1)-O(5)	130.0(5)

Na(3)-O(12)#14	2.756(10)	O(11)#3-Na(1)-O(7)#2	74.8(4)
Na(3)-O(12)#3	2.493(8)	O(11)#3-Na(1)-O(9)#2	96.1(4)
Na(4)-O(5)#17	2.996(10)	O(11)#3-Na(1)-O(10)#2	121.0(5)
Na(4)-O(6)#17	2.415(10)	O(11)#3-Na(1)-O(13)#2	75.4(4)
Na(4)-O(6)	2.341(10)	O(13)#2-Na(1)-O(2)#2	51.0(3)
Na(4)-O(11)#3	2.790(11)	O(2)#2-Li(2)-O(3)#2	64.8(6)
Na(4)-O(13)#2	2.354(10)	O(2)#2-Li(2)-O(7)#5	149.8(10)
Na(4)-O(13)#16	2.347(11)	O(2)#2-Li(2)-O(13)#4	93.2(7)
O(1)-B(1)	1.423(14)	O(3)#2-Li(2)-O(7)#5	85.0(7)
O(1)-B(2)	1.403(15)	O(3)#2-Li(2)-O(13)#4	152.5(9)
O(1)-Li(1A)	2.07(3)	O(6)#4-Li(2)-O(2)#2	97.1(8)
O(2)-Na(1)#6	2.935(13)	O(6)#4-Li(2)-O(3)#2	100.2(10)
O(2)-Li(2)#6	2.129(19)	O(6)#4-Li(2)-O(7)#5	88.3(8)
O(2)-B(2)	1.490(15)	O(6)#4-Li(2)-O(13)#4	64.7(5)
O(3)-P(1)#3	1.567(9)	O(7)#5-Li(2)-O(13)#4	115.7(7)
O(3)-Li(2)#6	2.26(2)	O(11)-Li(2)-O(2)#2	100.1(10)
O(3)-Na(2)#6	2.560(8)	O(11)-Li(2)-O(3)#2	112.0(8)
O(3)-B(2)	1.491(15)	O(11)-Li(2)-O(6)#4	147.6(10)
O(4)-Na(1)#6	2.691(13)	O(11)-Li(2)-O(7)#5	90.3(8)
O(4)-Na(2)#6	2.361(7)	O(11)-Li(2)-O(13)#4	87.0(9)
O(4)-B(2)	1.505(15)	O(8)-P(2)-O(4)	111.6(5)
O(5)-Na(4)#11	2.996(10)	O(8)-P(2)-O(9)	110.4(5)
O(5)-B(1)	1.452(16)	O(8)-P(2)-O(10)	114.2(4)
O(6)-Li(2)#10	2.11(2)	O(9)-P(2)-O(4)	103.6(3)
O(6)-Na(4)#11	2.415(10)	O(10)-P(2)-O(4)	108.3(5)
O(7)-Na(1)#6	2.492(13)	O(10)-P(2)-O(9)	108.2(5)
O(7)-Li(2)#8	2.27(2)	O(6)-P(3)-O(2)	111.4(5)
O(7)-B(1)	1.504(16)	O(6)-P(3)-O(7)	111.3(5)
O(7)-Li(1A)#6	2.30(3)	O(7)-P(3)-O(2)	103.3(4)
O(8)-Na(2)#7	2.410(9)	O(13)-P(3)-O(2)	108.2(5)
O(8)-Na(3)#9	2.459(10)	O(13)-P(3)-O(6)	114.1(5)
O(9)-Na(1)#6	2.649(13)	O(13)-P(3)-O(7)	108.0(5)
O(9)-Na(2)#8	2.378(8)	O(10)#2-Na(3)-O(10)#15	96.6(4)
O(9)-B(1)	1.494(14)	O(10)#2-Na(3)-O(12)#3	88.9(3)
O(10)-Na(1)#6	2.689(12)	O(10)#15-Na(3)-O(12)#14	102.7(3)
O(10)-Na(2)#7	2.579(8)	O(10)#15-Na(3)-O(12)#3	77.5(3)
O(10)-Na(3)#18	2.492(9)	O(10)#2-Na(3)-O(12)#14	73.3(3)
O(10)-Na(3)#6	2.460(9)	O(6)#17-Na(4)-O(5)#17	90.4(3)

O(11)-Na(1)#1	2.472(13)	O(6)-Na(4)-O(5)#17	86.2(3)
O(11)-Na(4)#1	2.790(11)	O(6)-Na(4)-O(6)#17	88.8(4)
O(11)-Li(1A)#1	2.20(4)	O(6)-Na(4)-O(11)#3	116.5(3)
O(12)-Na(3)#9	2.756(10)	O(6)#17-Na(4)-O(11)#3	87.8(3)
O(12)-Na(3)#1	2.493(8)	O(6)-Na(4)-O(13)#16	168.2(4)
O(13)-Na(1)#6	2.858(13)	O(6)-Na(4)-O(13)#2	89.1(3)
O(13)-Li(2)#10	2.536(19)	O(11)#3-Na(4)-O(5)#17	157.2(3)
O(13)-Na(4)#6	2.354(10)	O(13)#2-Na(4)-O(5)#17	105.8(3)
O(13)-Na(4)#12	2.347(11)	O(13)#16-Na(4)-O(5)#17	82.6(3)
O(13)-Li(1A)#6	2.31(5)	O(13)#16-Na(4)-O(6)#17	87.6(3)
O(3)#2-Na(2)-O(10)#13	152.7(3)	O(13)#2-Na(4)-O(6)#17	163.6(4)
O(4)#2-Na(2)-O(3)#2	58.3(3)	O(13)#16-Na(4)-O(11)#3	74.6(3)
O(4)#2-Na(2)-O(8)#13	110.5(3)	O(13)#2-Na(4)-O(11)#3	78.6(3)
O(4)#2-Na(2)-O(9)#5	132.3(3)	O(13)#16-Na(4)-O(13)#2	97.4(4)
O(4)#2-Na(2)-O(10)#13	100.4(3)	O(1)-B(1)-O(5)	108.9(10)
O(8)#13-Na(2)-O(3)#2	108.6(3)	O(1)-B(1)-O(7)	110.2(9)
O(8)#13-Na(2)-O(10)#13	60.1(3)	O(1)-B(1)-O(9)	111.7(9)
O(9)#5-Na(2)-O(3)#2	74.3(3)	O(5)-B(1)-O(7)	109.3(9)
O(9)#5-Na(2)-O(8)#13	87.9(3)	O(5)-B(1)-O(9)	112.2(9)
O(9)#5-Na(2)-O(10)#13	126.3(3)	O(9)-B(1)-O(7)	104.5(10)
O(12)-Na(2)-O(3)#2	113.8(3)	O(1)-B(2)-O(2)	111.9(10)
O(12)-Na(2)-O(4)#2	86.8(3)	O(1)-B(2)-O(3)	115.0(10)
O(12)-Na(2)-O(8)#13	137.0(3)	O(1)-B(2)-O(4)	111.6(9)
O(12)-Na(2)-O(9)#5	109.5(3)	O(2)-B(2)-O(3)	104.2(9)
O(12)-Na(2)-O(10)#13	78.7(3)	O(2)-B(2)-O(4)	106.9(9)
O(8)-Na(3)-O(8)#14	91.5(4)	O(3)-B(2)-O(4)	106.6(9)
O(8)-Na(3)-O(10)#2	88.5(3)	O(1)-Li(1A)-O(7)#2	172(2)
O(8)#14-Na(3)-O(10)#15	84.5(3)	O(1)-Li(1A)-O(11)#3	90.0(14)
O(8)#14-Na(3)-O(10)#2	166.0(3)	O(1)-Li(1A)-O(13)#2	109.7(18)
O(8)-Na(3)-O(10)#15	173.6(4)	O(7)#2-Li(1A)-O(13)#2	65.3(10)
O(8)-Na(3)-O(12)#3	106.5(3)	O(11)#3-Li(1A)-O(7)#2	84.2(8)
O(8)-Na(3)-O(12)#14	75.0(3)	O(11)#3-Li(1A)-O(13)#2	93.1(16)
O(8)#14-Na(3)-O(12)#3	77.6(3)		

Symmetry transformations used to generate equivalent atoms:

#1 $x-1,y,z$ #2 $x+1,y,z$ #3 $-x+3/2,y,z+1/2$ #4 $-x+1,-y+2,z+1/2$

#5 $-x+1/2,y,z+1/2$ #6 $-x+1,-y+1,z-1/2$ #7 $-x+1/2,y,z-1/2$

#8 $x-1/2,-y+1,z$ #9 $-x+3/2,y,z-1/2$ #10 $x-1/2,-y+2,z$

#11 $-x+2,-y+2,z-1/2$ #12 $-x+1,-y+1,z+1/2$ #13 $x+1/2,-y+1,z$

#14 $-x+2,-y+1,z+1/2$ #15 $-x+2,-y+2,z+1/2$ #16 $x+1/2,-y+2,z$
#17 $-x+1,-y+2,z-1/2$ #18 $-x+2,-y+1,z-1/2$