Synthesis and Characterizations of a New Rare Earth Borate Nonlinear Optical Crystal $K_7PbLu_2B_{15}O_{30}$

Juhe Liu,[a,c,d] Yuwei Chen, [a,b,d] Mengran Sun,[a,b,d] Wenhao Liu, [a,b,d], Xianghe Meng,[a,d*]and Jiyong Yao[a,b*]

[a] Beijing Center for Crystal Research and Development, Key Lab of Functional Crystals and Laser Technology, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, P. R. China.

[b] Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, P. R. China.

[c] School of Future Technology, University of Chinese Academy of Sciences, Beijing, 100049, China

[d] University of Chinese Academy of Sciences, Beijing 100049, P. R. China.

*Corresponding author:

Jiyong Yao; jyao@mail.ipc.ac.cn

Xianghe Meng: mengxianghe@mail.ipc.ac.cn

Table S1 Selected Bond Lengths for $K_7PbLu_2B_{15}O_{30}$

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Lu1	O1	2.182(6)	K1	O5[2]	2.705(6)
Lu1	O1[2]	2.182(6)	K1	O5[17]	2.705(6)
Lu1	O1[3]	2.182(6)	K1	O5[18]	2.705(6)
Lu1	O4[4]	2.296(7)	K1	O5[16]	2.706(6)
Lu1	O4[5]	2.295(7)	K1	O5	2.706(6)
Lu1	O4[6]	2.296(7)	K2	O1[16]	2.843(6)
Pb1	O4	2.503(7)	K2	O1[19]	2.843(6)
Pb1	O4[11]	2.503(7)	K2	O2[19]	3.211(8)
Pb1	O4[12]	2.503(7)	K2	O2[16]	3.211(8)
Pb1	O4[13]	2.503(7)	K2	O3[20]	2.931(7)
Pb1	O4[14]	2.503(7)	K2	O3[2]	2.931(7)
Pb1	O4[15]	2.503(7)	K2	O5[20]	2.778(6)
B1	O3[16]	1.454(11)	K2	O5[2]	2.778(6)
B1	O5[16]	1.473(11)	K3	O1[19]	2.797(6)
B3	O4[16]	1.346(13)	K3	O1[22]	2.797(6)
B2	O5[16]	1.370(12)	K3	O2[19]	3.222(7)
B2	O1	1.329(12)	K3	O2[22]	2. 222(7)
B2	O2	1.399(12)	K3	O3[23]	2.837(8)
B3	O2	1.413(12)	K3	O3[11]	2.837(8)
B3	O3	1.358(15)	K3	O4[17]	2.939(7)
K1	O5[3]	2.705(6)	K3	O4	2.939(7)

注：[2]-1-Y, +X-Y, +Z; [3]-1+Y-X, -1-X, +Z; [4]1/3-Y+X, -1/3-Y, 2/3-Z; [5]-2/3+Y, 2/3+X, 2/3-Z; [6]-5/3-X, -4/3-X+Y, 2/3-Z; [9]2/3+X, 1/3+Y, 1/3+Z; [11]-2+Y-X, -1-X, +Z; [12]-2-X, -1-X+Y, -Z; [13]-1-Y, 1+X-Y, +Z; [14]-1+Y, 1+X, -Z; [15]-Y+X, -Y, -Z; [16]-4/3-X, -2/3-X+Y, 1/3-Z; [17]-1/3-Y+X, -2/3-Y, 1/3-Z; [20]-1+Y, +X, -Z; [23]-4/3+Y, 1/3+X, 1/3-Z.

Table S2 Selected Bond Angles for $K_7PbLu_2B_{15}O_{30}$

Atom			Angle/°	Atom			Angle/°
O3[6]	B1	O3	109.2(11)	O3	B3	O2	118.4(9)
O3[16]	B1	O5[16]	108.7(3)	O4[16]	B3	O3	121.8(9)
O3	B1	O5	108.7(3)	O4[16]	B3	O2	119.7(11)
O3	B1	O5[16]	111.4(3)	B2	O2	B3	121.3(8)

O3[16]	B1	O5	111.4(3)	B3	O3	B1	125.5(7)
O5[16]	B1	O5	107.5(11)	B2	O1	Lu1	143.5(6)
O1	B2	O2	117.8(9)	B3[16]	O4	Lu1[9]	131.7(7)
O1	B2	O5[16]	123.4(8)	B2[16]	O5	B1	124.3(6)
O5[16]	B2	O2	118.8(8)				

注: [9]-2/3+Y, 2/3+X, 2/3-Z; [16]-4/3-X, -2/3-X+Y, 1/3-Z

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for $K_7PbLu_2B_{15}O_{30}$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Lu	12.6(2)	12.6(2)	10.5(3)	0	0	6.3(1)
Pb	26.3(3)	26.3(3)	16.8(3)	0	0	13.17(13)
O1	23(4)	21(3)	21(3)	6(2)	0(2)	14(3)
O2	30(5)	25(4)	41(4)	10(3)	-17(3)	3(3)
O3	29(4)	17(3)	24(3)	2(3)	-6(3)	10(3)
O4	25(4)	32(5)	44(4)	-9(3)	-4(3)	18(4)
O5	21(3)	25(3)	17(3)	-5(3)	-1(3)	14(3)
B1	27(8)	23(5)	16(7)	-1(3)	-3(6)	13(4)
B2	18(7)	17(4)	19(4)	-4(3)	3(4)	7(4)
B3	30(8)	17(4)	28(4)	-2(3)	-3(6)	16(5)
K1	18.6(11)	18.6(11)	43(3)	0	0	9.3(6)
K2	22.4(15)	32.4(12)	26.0(15)	-1.4(6)	-2.7(12)	11.2(8)
K3	21.0(17)	29.4(13)	36.3(14)	-14.3(11)	-7.2(6)	14.7(7)

Table S4 Atomic Coordinates ($×10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2×10^3$) for $K_7PbLu_2B_{15}O_{30}$.

Atom	*x*	*y*	*z*	U(eq)
Lu1	-6667	-3333	4400.6(3)	11.89(17)
Pb1	-10000	0	0	23.2(2)
O1	-5643(5)	-1696(5)	3669(4)	20.7(16)
O2	-4733(6)	76(6)	2888(5)	37(2)
O3	-5623(6)	354(5)	1616(4)	23.7(14)
O4	-9553(6)	-987(6)	1228(5)	32.1(18)
O5	-6700(5)	-1493(6)	888(4)	20.5(13)

B1	-6667	-811(12)	1667	22(3)
B2	-5695(10)	-1058(8)	3010(6)	19(3)
B3	-4707(14)	801(8)	2191(7)	23(3)
K1	-6667	-3333	1667	26.8(9)
K2	-10000	-4625(3)	0	28.1(7)
K3	-11532(3)	-3333	1667	28.0(8)

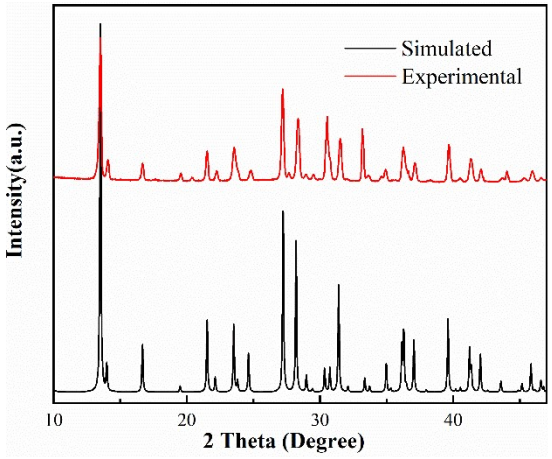

Fig. S1 Comparison of experimental polycrystalline powder and theoretically simulated PXRD patterns of $K_7PbLu_2B_{15}O_{30}$

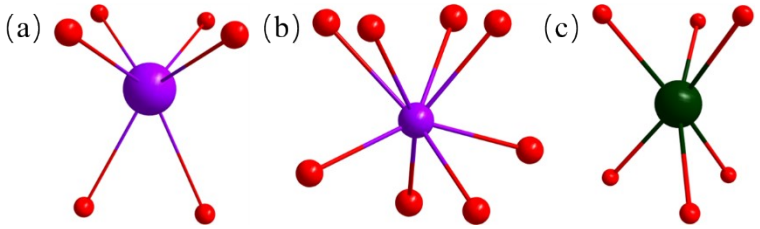

Fig. S2 (a) KO_6, (b) KO_8, and (c) PbO_6 groups.

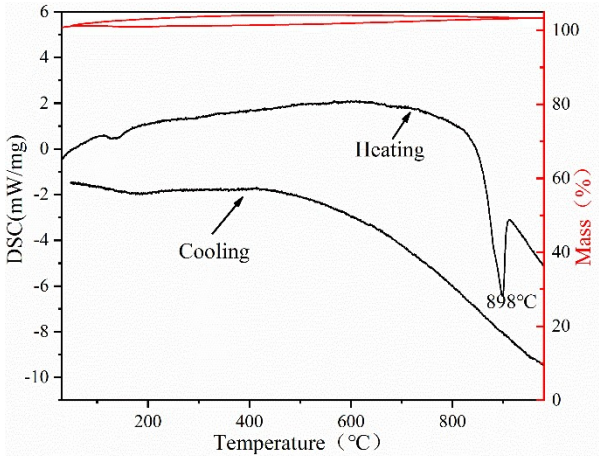

Fig. S3 DSC and TG curves of $K_7PbLu_2B_{15}O_{30}$

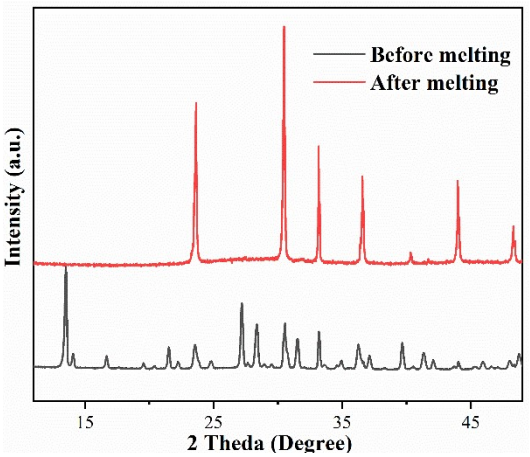

Fig. S4 Comparison diagram of XRD before and after melting of compound $K_7PbLu_2B_{15}O_{30}$

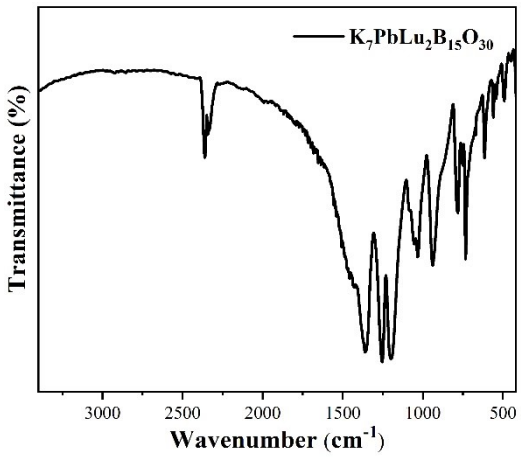

Fig. S5 IR spectra for $K_7PbLu_2B_{15}O_{30}$