SUPPORTING INFORMATION

$K_7MgY_2(B_5O_{10})_3$: A novel ultraviolet nonlinear optical crystal based on the $[B_5O_{10}]$ functional unit

Haozhen Liu[a], Shiyu Du[a], Paipai Zhang[b], Jiawei Zhao[a], Yanna Chen*[a] and Donghai An*[a,]

[a]School of Physics and Materials Science, Changji University, Changji 831100, People's Republic of China.

[b]School of Physics and Technology, Xinjiang University, Urumqi 830000, People's Republic of China.

*Corresponding Author(s): adhcjxy@163.com and ynchenaa@163.com.

Title

Figure S1. Powder XRD patterns for $K_7MgY_2(B_5O_{10})_3$.

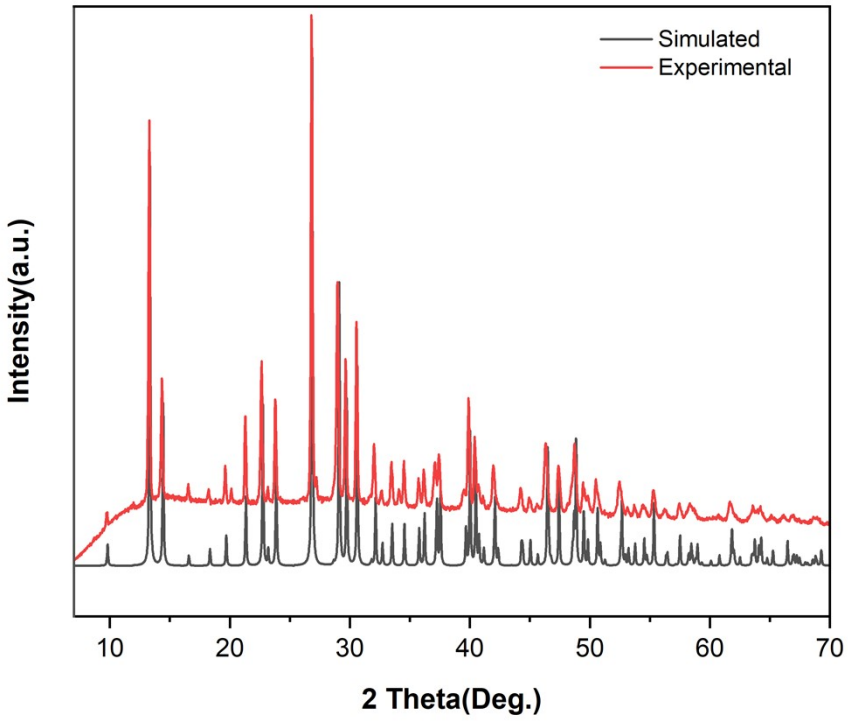
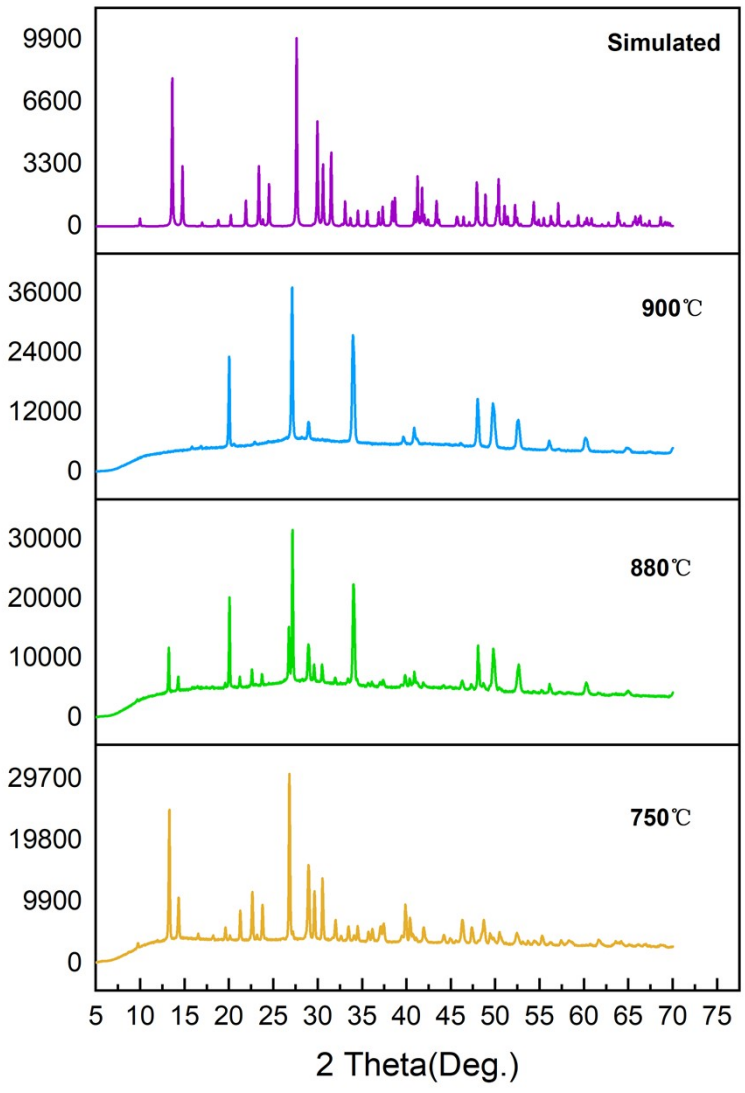


Table S1. A summary of reported RE-based NLO crystals with $[B_5O_{10}]^{5-}$ groups.

Molecular formula	NLO motifs	Space	Cutoff	SHG	PM
$Rb_7SrSc_2(B_5O_{10})_3$[1]	$[B_5O_{10}]$+$[ScO_6]$	*R32*		0.76	NO
$Rb_7CaSc_2(B_5O_{10})_3$[1]	$[B_5O_{10}]$+$[ScO_6]$	*R32*		0.88	NO
$K_7PbLu_2(B_5O_{10})_3$[2]	$[B_5O_{10}]$+$[LuO_6]$	*R32*		1.1	YES
$Rb_7CaY_2(B_5O_{10})_3$[3]	$[B_5O_{10}]$+$[YO_6]$	*R32*		1.4	YES
$K_6NaSrSc_2(B_5O_{10})_3$[4]	$[B_5O_{10}]$+$[ScO_6]$	*R32*	248	0.7	YES
$K_6LiCaSc_2(B_5O_{10})_3$[5]	$[B_5O_{10}]$+$[ScO_6]$	*R32*		0.4	YES
$K_6NaCaSc_2(B_5O_{10})_3$[5]	$[B_5O_{10}]$+$[ScO_6]$	*R32*		0.4	YES
$K_6Li_{0.7}Na_{0.3}CaSc_2(B_5O_{10})_3$[5]	$[B_5O_{10}]$+$[ScO_6]$	*R32*		0.4	YES
$Rb_6NaCaY_2(B_5O_{10})_3$[3]	$[B_5O_{10}]$+$[YO_6]$	*R32*		1.2	YES

Figure S2. Post-heating XRD analysis for $K_7MgY_2(B_5O_{10})_3$.



$Rb_6LiCaY_2(B_5O_{10})_3$[3]	$[B_5O_{10}]+[YO_6]$	*R32*		1.1	NO
$K_7CdLu_2(B_5O_{10})_3$[6]	$[B_5O_{10}]+[LuO_6]$	*R32*	192	1.9	YES
$K_7PbY_2(B_5O_{10})_3$[6]	$[B_5O_{10}]+[YO_6]$	*R32*	N/A	2.1	YES
$K_7PbSc_2(B_5O_{10})_3$[6]	$[B_5O_{10}]+[ScO_6]$	*R32*	N/A	N/A	N/A
$K_7PbGd_2(B_5O_{10})_3$[6]	$[B_5O_{10}]+[GdO_6]$	*R32*	N/A	N/A	N/A
$K_7ZnSc_2(B_5O_{10})_3$[6]	$[B_5O_{10}]+[ScO_6]$	*R32*	N/A	N/A	N/A
$K_7Zn_{0.69}Pb_{0.31}Gd_2(B_5O_{10})_3$[6]	$[B_5O_{10}]+[GdO_6]$	*R32*	N/A	N/A	N/A
$K_7Zn_{0.77}Pb_{0.23}Gd_2(B_5O_{10})_3$[6]	$[B_5O_{10}]+[GdO_6]$	*R32*	N/A	N/A	N/A
$K_7Cd_{0.89}Pb_{0.11}Lu_2(B_5O_{10})_3$[6]	$[B_5O_{10}]+[LuO_6]$	*R32*	N/A	N/A	N/A
$K_7Cd_{0.85}Pb_{0.15}Lu_2(B_5O_{10})_3$[6]	$[B_5O_{10}]+[LuO_6]$	*R32*	N/A	N/A	N/A
$Rb_7SrY_2(B_5O_{10})_3$[7]	$[B_5O_{10}]+[YO_6]$	*R32*		0.9	NO
$Rb_7SrGd_2(B_5O_{10})_3$[8]	$[B_5O_{10}]+[GdO_6]$	*R32*		0.5	NO
$K_7CaY_2(B_5O_{10})_3$[9]	$[B_5O_{10}]+[YO_6]$	*R32*		0.9	YES
$K_7SrY_2(B_5O_{10})_3$[9]	$[B_5O_{10}]+[YO_6]$	*R32*		1.1	YES
$K_7BaY_2(B_5O_{10})_3$[9]	$[B_5O_{10}]+[YO_6]$	*R32*		1.2	YES
$K_7CaLu_2(B_5O_{10})_3$[9]	$[B_5O_{10}]+[LuO_6]$	*R32*	N/A	N/A	N/A
$K_7SrLu_2(B_5O_{10})_3$[9]	$[B_5O_{10}]+[LuO_6]$	*R32*	N/A	N/A	N/A
$K_7BaLu_2(B_5O_{10})_3$[9]	$[B_5O_{10}]+[LuO_6]$	*R32*	N/A	N/A	N/A
$K_7CaGd_2(B_5O_{10})_3$[9]	$[B_5O_{10}]+[GdO_6]$	*R32*	N/A	N/A	N/A
$K_7SrGd_2(B_5O_{10})_3$[9]	$[B_5O_{10}]+[GdO_6]$	*R32*	N/A	N/A	N/A
$K_7CdSc_2(B_5O_{10})_3$[6]	$[B_5O_{10}]+[ScO_6]$	*R32*		1.5	YES
$K_7CdY_2(B_5O_{10})_3$[6]	$[B_5O_{10}]+[YO_6]$	*R32*		1.6	YES
$K_7CdGd_2(B_5O_{10})_3$[6]	$[B_5O_{10}]+[GdO_6]$	*R32*	206	1.7	YES
$K_7MgSc_2(B_5O_{10})3$	$[B_5O_{10}]+[ScO_6]$	*R32*	<190	0.9	YES
$K_7Sr_{0.34}Sc_{2.44}(B_5O_{10})_3$	$[B_5O_{10}]+[ScO_6]$	*R32*	<190	N/A	N/A
$K_6Li_{0.94}BaY_{2.02}(B_5O_{10})_3$	$[B_5O_{10}]+[YO_6]$	*R32*	<190	N/A	N/A
$K_6NaBaY_2(B_5O_{10})_3$	$[B_5O_{10}]+[YO_6]$	*R32*	<190	N/A	N/A
$Rb_{5.3}Na_{3.7}Y_2(B_5O_{10})_3$	$[B_5O_{10}]+[YO_6]$	*R32*	<190	N/A	N/A
$Rb_6Na_{1.5}Y_{2.5}(B_5O_{10})_3$	$[B_5O_{10}]+[YO_6]$	*R32*	<190	1.3	YES
$K_6Na_{1.82}Y_{2.18}(B_5O_{10})_3$	$[B_5O_{10}]+[YO_6]$	*R32*	<190	N/A	N/A
$K_7Mg_{0.88}Zn_{0.12}Y_2(B_5O_{10})_3$	$[B_5O_{10}]+[YO_6]$	*R32*	<190	1.2	YES
$Rb_6LiCaY_2(B_5O_{10})_3$	$[B_5O_{10}]+[YO_6]$	$C222_1$	<190	N/A	N/A
$K_6NaSrY_2(B_5O_{10})_3$	$[B_5O_{10}]+[YO_6]$	*R32*	< 200	0.9	YES
$Rb_7BaLu_2(B_5O_{10})_3$	$[B_5O_{10}]+[LuO_6]$	*R32*	< 200	1.2	YES
$K_7PbLu_2(B_5O_{10})_3$	$[B_5O_{10}]+[LuO_6]$	*R32*	< 200		N/A
$K_6NaCaY_2(B_5O_{10})_3$	$[B_5O_{10}]+[YO_6]$	*R32*	230	0.5	YES
$K_6NaCaLu_2(B_5O_{10})_3$	$[B_5O_{10}]+[LuO_6]$	*R32*	236	0.5	YES

Table S2. Atomic coordinates, equivalent isotropic displacement parameters(Å2), and bond valence sum (BVS) for $K_7MgY_2(B_5O_{10})_3$.

Atom	x	y	z	U(eq)
Y1	10000	10000	7153.0(3)	7.51(11)
Mg1	6667	3333	8333	4.7(4)
K1	5103.0(9)	5103.0(9)	10000	30.0(3)
K2	6667	7960.9(7)	8333	19.5(2)
K3	10000	10000	10000	21.2(3)
B1	8157(3)	5821(3)	9335(2)	14.5(7)
B2	9059(3)	7725(2)	8582(2)	11.0(7)
B3	10000	7481(3)	10000	13.1(10)
O1	8951.7(15)	8389.9(15)	7943.8(13)	13.2(4)
O2	8186(2)	6560.0(14)	8635.7(14)	25.6(5)
O3	8959.3(16)	6317.4(15)	10038.7(12)	15.4(4)
O4	7382(2)	4700.8(13)	9330.6(11)	19.0(4)
O5	9975.4（16）	8126.3(16)	9183.5(12)	13.1(4)

Table S3. Bond lengths (Å) for $K_7MgY_2(B_5O_{10})_3$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
K1	$O1^{10}$	2.7171(19)	K3	O5	2.7391(19)
K1	$O1^{14}$	2.7171(19)	K3	$O5^{5}$	2.7391(19)
K1	$O2^{14}$	2.857(2)	Mg1	$O4^{8}$	2.1356(16)
K1	$O2^{10}$	2.857(2)	Mg1	$O4^{9}$	2.1355(16)
K1	$O3^{11}$	2.840(2)	Mg1	$O4^{10}$	2.1355(16)
K1	$O3^{13}$	2.840(2)	Mg1	O4	2.1355(16)
K2	O1	2.8480(17)	Mg1	$O4^{11}$	2.1355(16)
K2	$O1^{10}$	2.8480(18)	Mg1	$O4^{12}$	2.1356(16)
K2	$O2^{10}$	3.385(3)	Y1	$O1^{5}$	2.2003(18)
K2	O2	3.385(3)	Y1	O1	2.2003(18)
K2	$O3^{2}$	2.855(2)	Y1	$O1^{4}$	2.2003(18)
K2	$O3^{15}$	2.855(2)	Y1	$O4^{1}$	2.2973(16)
K2	$O5^{16}$	2.7392(19)	Y1	$O4^{3}$	2.2974(16)
K2	$O5^{4}$	2.7393(19)	Y1	$O4^{2}$	2.2973(16)
K3	$O5^{17}$	2.7391(19)	B3	O3	1.471(3)
K3	$O5^{18}$	2.7391(19)	B3	O5	1.470(3)
K3	$O5^{15}$	2.7391(19)			
K3	$O5^{4}$	2.7391(19)			

Table S4.Bond angles (deg.) for $K_7MgY_2(B_5O_{10})_3$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1[11]	K1	O1[14]	172.14(9)	O5	K3	O5[15]	125.25(8)
O1[11]	K1	O2[14]	130.51(5)	O5[4]	K3	O5	102.71(5)
O1[14]	K1	O2[11]	130.51(5)	O5[17]	K3	O5[5]	51.21(8)
O1[14]	K1	O2[14]	49.83(5)	O5	K3	O5[18]	51.21(7)
O1[11]	K1	O2[11]	49.53(5)	O5[4]	K3	O5[5]	102.71(5)
O1[11]	K1	O3[13]	75.03(5)	O5[5]	K3	O5[18]	125.25(8)
O1[14]	K1	O3[12]	75.03(5)	O5	K3	O5[5]	102.71(5)
O1[14]	K1	O3[13]	112.49(6)	O5[17]	K3	O5	127.54(8)
O1[11]	K1	O3[12]	112.49(6)	O5[15]	K3	O5[5]	127.54(8)
O3[12]	K1	O2[11]	89.89(7)	O5[17]	K3	O5[18]	102.71(4)
O3[13]	K1	O2[14]	89.89(7)	O4[12]	Mg1	O4[9]	177.72(16)
O3[13]	K1	O2[11]	89.70(7)	O4[11]	Mg1	O4[8]	79.21(7)
O3[13]	K1	O3[12]	49087(8)	O4[11]	Mg1	O4[9]	79.21(7)
O1[11]	K2	O1	141.16(8)	O4[8]	Mg1	O4[9]	79.21(7)
O1[11]	K2	O2	99.68(6)	O4	Mg1	O4[8]	177.72(16)
O1	K2	O2	43.00(5)	O4[11]	Mg1	O4[10]	177.72(16)
O1[11]	K2	O2[11]	43.00(5)	O4	Mg1	O4[12]	79.22(7)
O1	K2	O2[11]	99.68(6)	O4[11]	Mg1	O4	102.29(12)
O1	K2	O3[2]	83.56(5)	O4	Mg1	O4[9]	99.33(12)
O1[11]	K2	O3[15]	83.56(5)	O4[10]	Mg1	O4	79.22(12)
O1[11]	K2	O3[2]	118.34(5)	O4[12]	Mg1	O4[8]	102.29(12)
O1	K2	O3[15]	118.34(5)	O1[5]	Y1	O1	95.34(7)
O2	K2	O2[11]	64.24(7)	O1[5]	Y1	O1[4]	95.34(7)
O3[2]	K2	O2[11]	115.29(5)	O1[4]	Y1	O1	95.34(7)
O3[15]	K2	O2	115.29(5)	O1[5]	Y1	O4[2]	163.29(7)
O3[15]	K2	O2[11]	119.75(6)	O1[5]	Y1	O4[1]	99.46(8)
O3[2]	K2	O2	119.75(6)	O1	Y1	O4[1]	163.29(7)
O5[17]	K3	O5[15]	102.71(4)	O1[4]	Y1	O4[3]	163.29(7)
O5[4]	K3	O5[18]	127.54(8)	O1[4]	Y1	O4[1]	91.00(7)
O5[17]	K3	O5[4]	125.25(8)	O1[5]	Y1	O4[3]	91.00(7)
O5[4]	K3	O5[15]	51.21(7)	O1	Y1	O4[32]	91.00(7)
O5[15]	K3	O5[18]	102.71(5)	O1	Y1	O4[3]	99.46(8)

[1]1/3+X,2/3+Y,-1/3+Z; [2]4/3-Y,2/3+X-Y,-1/3+Z; [3]4/3+Y-X,5/3-X,-1/3+Z; [4]1+Y-X,2-X,+Z; [5]2-Y,1+X-Y,+Z; [6]-1/3+Y,-2/3+X,4/3-Z; [7]-1/3+X,-2/3+Y,1/3+Z; [8]1/3-Y+X,2/3-Y,5/3-Z; [9]1/3+Y,-1/3+X,5/3-Z; [10]1+Y-X,1-X,+Z; [11]4/3-X,2/3-X+Y,5/3-Z; [12]1-Y,+X-Y,+Z; [13]-Y+X,1-Y,2-Z; [14]2/3+Y-X,4/3-X,1/3+Z; [15]+Y,+X,2-Z; [16]1/3-Y+X,5/3-Y,5/3-Z; [17]1-Y+X,2-Y,2-Z; [18]2-X,1-X+Y,2-Z

References

(1) Liu, W.; Lee, M.-H.; Guo, R.; Yao, J. Two Non-Centrosymmetric Mixed Alkali Metal and Alkaline Earth Metal Scandium Borate Nonlinear Optical Materials with Short Ultravio let Cutoff Edges. *Dalton Trans*. **2023**, 52 (11), 3344–3350.

(2) Liu, J.; Chen, Y.; Sun, M.; Liu, W.; Meng, X.; Yao, J. Synthesis and Characterization of a New Rare Earth Borate Nonlinear Optical Crystal $K_7PbLu_2B_{15}O_{30}$. *Dalton Trans*. **202 3**, 52 (29), 10109–10114.

(3) Wu, C.; Dang, Y.; Chen, J.; Hou, X.; Shi, H. Three Borates Belonging to the $A(I)_7Ae(II)Re(III)_2B_{15}O_{30}$ Family as Promising Nonlinear Optical Crystals. *Cryst. Growth Des*. **202 3**, 23 (9), 6885–6893.

(4) Liu, W.; Liu, X.; Meng, X.; Li, C.; Sun, M.; Lin, Z.; Yao, J. Two Non-Centrosymme tric Scandium Borate Nonlinear Optical Crystals Containing the B_5O_{10} Anion Group. *J. All oys Compd*. **2022**, 902 (163832), 163832.

(5) Feng, J.; Xu, X.; Hu, C.; Mao, J. $K_6ACaSc_2(B_5O_{10})_3$ (A = Li, Na, Li0.7Na0.3): Nonli near-Optical Materials with Short UV Cutoff Edges. *Inorg. Chem*. **2019**, 58 (4), 2833–283 9.

(6) Xie, Z.; Mutailipu, M.; He, G.; Han, G.; Wang, Y.; Yang, Z.; Zhang, M.; Pan, S. A Series of Rare-Earth Borates $K_7MRE_2B_{15}O_{30}$ (M = Zn, Cd, Pb; RE = Sc, Y, Gd, Lu) with Large Second Harmonic Generation Responses. *Chem. Mater*. **2018**, 30(7), 2414–2423.

(7) Li, Y.; Liang, F.; Song, H.; Liu, W.; Lin, Z.; Zhang, G.; Wu, Y. $Rb_7SrY_2(B_5O_{10})_3$: A Rare-Earth Pentaborate with Moderate Second-Harmonic Response and Interesting Phase-Ma tching Behavior. *Inorg. Chem*. **2019**, 58 (14), 8943–8947.

(8) Liu, W.; Liu, X.; Shen, J.; Li, Y.; Song, H.; Feng, J.; Lin, Z.; Zhang, G. A New No n-Centrosymmetric Gd-Based Borate Crystal $Rb_7SrGd_2(B_5O_{10})_3$: Growth, Structure, and Non linear Optical and Magnetic Properties. *Dalton Trans*. **2020**, 49 (27), 9355–9361.

(9) Mutailipu, M.; Xie, Z.; Su, X.; Zhang, M.; Wang, Y.; Yang, Z.; Janjua, M. R. S. A.; Pan, S. Chemical Cosubstitution-Oriented Design of Rare-Earth Borates as Potential Ultravi olet Nonlinear Optical Materials. *J. Am. Chem. Soc*. **2017**, 139 (50), 18397–18405.