Electronic Supplementary Material (ESI) for Dalton Transactions.

Novel red phosphors $KBaEu(XO_4)_3$ (X=Mo, W) show high color purity and high thermostability from a disorder chained structure

G. Q. Wang*[a,b], X. H. Gong[b], Y. J. Chen[b], J. H. Huang[b], Y. F. Lin[b], Z. D. Luo[b], and Y. D. Huang[b]

[a]*College of Materials Science and Engineering, Fuzhou University, Fuzhou, Fujian 350108, People's Republic of China.*

[b] *Key Laboratory of Optoelectronic Materials Chemistry and Physics, Fujian institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China.*

E-mail: gqwang@fzu.edu.cn.

CONTENTS

Table S1. Atomic coordinates and equivalent isotropic displacement parameters for $KBaEu(MoO_4)_3$ and $KBaEu(WO_4)_3$.

Compound	Atom	Wyck.	Site	x	y	z	U_{eq}[Å^2][a]
$KBaEu(MoO_4)_3$	Eu	4e	2	0	0.8815(1)	0.2500	0.0006(1)
	Mo(1)	8f	1	0.1569(1)	0.8892(1)	-0.997(1)	0.0007(1)
	Mo(2)	4e	2	0	0.6495(1)	-0.2500	0.0007(1)
	K	8f	1	-0.1648(1)	0.6251(1)	0.0758(1)	0.0011(1)
	Ba	8f	1	-0.1648(1)	0.6251(1)	0.0758(1)	0.0011(1)
	O(1)	8f	1	0.0781(2)	0.5663(2)	-0.749(6)	0.0016(1)
	O(2)	8f	1	0.0764(2)	0.9613(2)	-0.3429(5)	0.0009(1)
	O(3)	8f	1	0.2302(2)	0.9688(2)	0.1121(5)	0.0014(1)
	O(4)	8f	1	0.2061(2)	0.8012(2)	-0.2564(5)	0.0013(1)
	O(5)	8f	1	0.1125(2)	0.8123(2)	0.1049(5)	0.0011(1)
	O(6)	8f	1	-0.0394(2)	0.7288(3)	-0.0341(7)	0.0012(1)
Compound	Atom	Wyck.	Site	x	y	z	U_{eq}[Å^2][a]
$KBaEu(WO_4)_3$	Eu	4e	2	0	0.8794(1)	0.2500	0.0007(1)
	W(1)	8f	1	0.1574(1)	0.8913(1)	-0.1000(1)	0.0009(1)
	W(2)	4e	2	0	0.6476(1)	-0.2500	0.0009(1)
	K	8f	1	0.1656(6)	0.6247(9)	-0.5777(20)	0.0012(1)
	Ba	8f	1	0.1656(6)	0.6247(9)	-0.5777(20)	0.0012(1)
	O(1)	8f	1	0.0769(3)	0.9623(5)	-0.3456(12)	0.0011(1)
	O(2)	8f	1	0.2713(3)	0.5297(5)	-0.1286(12)	0.0020(2)
	O(3)	8f	1	0.1110(3)	0.8109(5)	0.0958(12)	0.0013(1)
	O(4)	8f	1	-0.0403(3)	0.7280(5)	-0.0343(12)	0.0015(1)
	O(5)	8f	1	-0.0777(3)	0.4357(5)	-0.9294(13)	0.0019(2)
	O(6)	8f	1	0.2071(3)	0.8018(5)	-0.2548(13)	0.0016(1)

[a] U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Table S2. Selected bond distances (Å) of $KBaEu(MoO_4)_3$ and $KBaEu(WO_4)_3$.

$KBaEu(MoO_4)_3$					
Eu—O6	2.385(3)	Mo1—O4	1.732(3)	K|Ba—O4iii	2.719(3)
Eu—O6i	2.385(3)	Mo1—O3	1.747(3)	K|Ba—O6	2.732(3)
Eu—O2ii	2.416(3)	Mo1—O5	1.777(3)	K|Ba—O1i	2.767(3)
Eu—O2iii	2.416(3)	Mo1—O2	1.848(3)	K|Ba—O1x	2.790(3)
Eu—O5	2.451(3)	Mo2—O1iii	1.746(3)	K|Ba—O4xi	2.794(3)
Eu—O5i	2.451(3)	Mo2—O1	1.746(3)	K|Ba—O5i	2.852(3)
Eu—O2iv	2.469(3)	Mo2—O6	1.785(3)	K|Ba—O3xii	2.876(3)
Eu—O2v	2.469(3)	Mo2—O6iii	1.785(3)	K|Ba—O3ix	2.692(3)
$KBaEu(WO_4)_3$					
Eu—O4	2.374(6)	W1—O6	1.740(6)	Ba|K—O2xiii	2.708(6)
Eu—O4i	2.374(6)	W1—O2vi	1.775(6)	Ba|K—O6	2.736(6)
Eu—O1ii	2.435(6)	W1—O3	1.785(6)	Ba|K—O4iii	2.736(6)
Eu—O1iii	2.435(6)	W1—O1	1.860(6)	Ba|K—O5xiv	2.766(7)
Eu—O3i	2.458(5)	W2—O5x	1.759(6)	Ba|K—O6viii	2.769(6)
Eu—O3	2.458(6)	W2—O5xi	1.759(6)	Ba|K—O5xii	2.781(6)
Eu—O1iv	2.487(6)	W2—O4iii	1.799(6)	Ba|K—O2	2.849(6)
Eu—O1v	2.487(6)	W2—O4	1.799(6)	Ba|K—O3vii	2.864(6)

Symmetry codes: (i) -x, y, 0.5-z; (ii) x, y, 1+z; (iii) -x, y, -0.5-z; (iv) x, 2-y, 0.5+z; (v) -x, 2-y, -z; (vi) 0.5-x, 1.5-y, -z; (vii) x, y, -1+z; (viii) 0.5-x, 1.5-y, -1-z; (ix) 0.5-x, 0.5+y, -0.5-z; (x) -x, 1-y, -1-z; (xi) x, 1-y, 0.5+z; (xii) -x, y, -1.5-z; (xiii) x, 1-y, -0.5+z; (xiv) -x, 1-y, -2-z.

Table S3. Selected Bond Angles (deg) for $KBaEu(MoO_4)_3$ and $KBaEu(WO_4)_3$.

$KBaEu(MoO_4)_3$			
O6—Eu—O6i	76.79(14)	O4—Mo1—O3	106.83(14)
O6—Eu—O2ii	151.41(10)	O4—Mo1—O5	109.17(14)
O6i—Eu—O2ii	75.88(9)	O3—Mo1—O5	105.23(12)
O6—Eu—O2iii	75.88(9)	O4—Mo1—O2	109.78(12)
O6i—Eu—O2iii	151.41(10)	O3—Mo1—O2	117.48(13)
O2ii—Eu—O2iii	132.27(13)	O5—Mo1—O2	108.08(12)
O6—Eu—O5	68.90(9)	O1iii—Mo2—O1	108.7(2)
O6i—Eu—O5	79.53(9)	O1iii—Mo2—O6	106.32(13)
O2ii—Eu—O5	97.88(9)	O1—Mo2—O6	110.74(13)
O2iii—Eu—O5	98.19(9)	O1iii—Mo2—O6iii	110.74(13)
O6—Eu—O5i	79.53(9)	O1—Mo2—O6iii	106.32(13)
O6i—Eu—O5i	68.90(9)	O6—Mo2—O6iii	113.98(19)
O2ii—Eu—O5i	98.19(9)	O3ix—K|Ba—O4iii	122.92(9)
O2iii—Eu—O5i	97.88(9)	O3ix—K|Ba—O6	161.35(9)
O5—Eu—O5i	139.57(13)	O4iii—K|Ba—O6	65.34(8)
O6—Eu—O2iv	123.90(9)	O3ix—K|Ba—O1i	86.79(9)
O6i—Eu—O2iv	131.63(9)	O4iii—K|Ba—O1i	142.02(9)
O2ii—Eu—O2iv	70.94(6)	O6—K|Ba—O1i	94.31(9)
O2iii—Eu—O2iv	72.28(11)	O3ix—K|Ba—O1x	77.40(9)
O5—Eu—O2iv	71.45(9)	O4iii—K|Ba—O1x	135.55(8)
O5i—Eu—O2iv	148.98(9)	O6—K|Ba—O1x	85.67(9)
O6—Eu—O2v	131.63(9)	O1i—K|Ba—O1x	68.51(8)
O6i—Eu—O2v	123.90(9)	O3ix—K|Ba—O4xi	65.31(9)
O2ii—Eu—O2v	72.28(11)	O4iii—K|Ba—O4xi	81.36(8)
O2iii—Eu—O2v	70.94(6)	O6—K|Ba—O4xi	133.10(8)
O5—Eu—O2v	148.98(9)	O1i—K|Ba—O4xi	92.60(8)
O5i—Eu—O2v	71.45(9)	O1x—K|Ba—O4xi	139.20(9)
O2iv—Eu—O2v	77.55(13)	O3ix—K|Ba—O5i	129.68(8)
O4xi—K|Ba—O5i	72.49(8)	O4iii—K|Ba—O5i	73.84(8)
O3ix—K|Ba—O3xii	59.79(6)	O6—K|Ba—O5i	67.26(8)
O4iii—K|Ba—O3xii	77.51(8)	O1i—K|Ba—O5i	68.62(8)
O6—K|Ba—O3xii	110.78(8)	O1x—K|Ba—O5i	126.47(8)
O1i—K|Ba—O3xii	140.39(8)	O4xi—K|Ba—O3xii	91.78(8)
O1x—K|Ba—O3xii	82.90(8)	O5i—K|Ba—O3xii	148.97(8)
$KBaEu(WO_4)_3$			
O4—Eu—O4i	77.8(3)	O6—W1—O2vi	108.6(3)
O4—Eu—O1ii	152.6(2)	O6—W1—O3	107.6(3)
O4i—Eu—O1ii	76.0(2)	O2vi—W1—O3	104.1(3)
O4—Eu—O1iii	76.0(2)	O6—W1—O1	109.8(3)
O4i—Eu—O1iii	152.6(2)	O2vi—W1—O1	119.3(3)
O1ii—Eu—O1iii	130.9(3)	O3—W1—O1	106.9(3)
O4—Eu—O3i	79.9(2)	O5x—W2—O5xi	109.5(4)

O4i—Eu—O3i	69.25(18)	O5x—W2—O4iii	106.4(3)
O1ii—Eu—O3i	98.1(2)	O5xi—W2—O4iii	110.3(3)
O1iii—Eu—O3i	98.12(19)	O5x—W2—O4	110.3(3)
O4—Eu—O3	69.25(18)	O5xi—W2—O4	106.4(3)
O4i—Eu—O3	79.9(2)	O4iii—W2—O4	113.9(4)
O1ii—Eu—O3	98.12(19)	O2xiii—Ba|K—O6	122.75(18)
O1iii—Eu—O3	98.1(2)	O2xiii—Ba|K—O4iii	162.60(19)
O3i—Eu—O3	140.2(3)	O6—Ba|K—O4iii	65.81(17)
O4—Eu—O1iv	123.8(2)	O2xiii—Ba|K—O5xiv	86.45(18)
O4i—Eu—O1iv	130.68(19)	O6—Ba|K—O5xiv	142.63(18)
O1ii—Eu—O1iv	70.09(12)	O4iii—Ba|K—O5xiv	93.34(18)
O1iii—Eu—O1iv	72.3(2)	O2xiii—Ba|K—O6viii	63.84(18)
O3i—Eu—O1iv	148.93(18)	O6—Ba|K—O6viii	81.35(19)
O3—Eu—O1iv	70.83(18)	O4iii—Ba|K—O6viii	133.44(18)
O4—Eu—O1v	130.68(19)	O5xiv—Ba|K—O6viii	93.88(19)
O4i—Eu—O1v	123.8(2)	O2xiii—Ba|K—O5xii	79.71(19)
O1ii—Eu—O1v	72.3(2)	O6—Ba|K—O5xii	134.35(18)
O1iii—Eu—O1v	70.09(12)	O4iii—Ba|K—O5xii	84.10(18)
O3i—Eu—O1v	70.83(18)	O5xiv—Ba|K—O5xii	67.94(15)
O3—Eu—O1v	148.93(18)	O6viii—Ba|K—O5xii	140.48(19)
O1iv—Eu—O1v	78.1(2)	O2xiii—Ba|K—O2	59.71(12)
O6—Ba|K—O3vii	75.31(18)	O6—Ba|K—O2	77.85(19)
O4iii—Ba|K—O3vii	67.26(18)	O4iii—Ba|K—O2	112.30(18)
O5xiv—Ba|K—O3vii	67.89(17)	O5xiv—Ba|K—O2	139.47(19)
O6viii—Ba|K—O3vii	73.27(16)	O6viii—Ba|K—O2	90.44(17)
O5xii—Ba|K—O3vii	124.81(17)	O5xii—Ba|K—O2	83.49(18)
O2—Ba|K—O3vii	150.32(17)	O2xiii—Ba|K—O3vii	127.94(18)

Symmetry codes: (i) -x, y, 0.5-z; (ii) x, y, 1+z; (iii) -x, y, -0.5-z; (iv) x, 2-y, 0.5+z; (v) -x, 2-y, -z; (vi) 0.5-x, 1.5-y, -z; (vii) x, y, -1+z; (viii) 0.5-x, 1.5-y, -1-z; (ix) 0.5-x, 0.5+y, -0.5-z; (x) -x, 1-y, -1-z; (xi) x, 1-y, 0.5+z; (xii) -x, y, -1.5-z; (xiii) x, 1-y, -0.5+z; (xiv) -x, 1-y, -2-z.

Table S4. Anisotropic displacement parameters (Å²) for $KBaEu(MoO_4)_3$ and $KBaEu(WO_4)_3$.

Compound	Atom	U11	U22	U33	U12	U13	U23
$KBaEu(MoO_4)_3$	Eu	0.0070(3)	0.0037(3)	0.0069(2)	0	0.00197(17)	0
	Mo1	0.0051(3)	0.0063(3)	0.0087(3)	0.00083(13)	0.0007(2)	0.00134(12)
	Mo2	0.0095(4)	0.0041(3)	0.0096(3)	0	0.0042(2)	0
	K	0.0096(4)	0.0074(3)	0.0163(3)	-0.00172(16)	0.0037(2)	0.00077(16)
	Ba	0.0096(4)	0.0074(3)	0.0163(3)	-0.00172(16)	0.0037(2)	0.00077(16)
	O1	0.0181(18)	0.0126(17)	0.0168(15)	0.0040(13)	0.0023(13)	0.0002(12)
	O2	0.0096(15)	0.0070(16)	0.0094(13)	0.0017(11)	0.0011(11)	-0.0004(11)
	O3	0.0145(16)	0.0125(17)	0.0131(14)	-0.0055(13)	0.0035(12)	0.0004(12)
	O4	0.0116(16)	0.0136(17)	0.0160(14)	-0.0004(12)	0.0060(12)	-0.0009(12)
	O5	0.0093(15)	0.0107(16)	0.0137(14)	0.0004(12)	0.0052(11)	0.0016(11)
	O6	0.0096(17)	0.0124(16)	0.0155(14)	-0.0037(12)	0.0054(12)	-0.0055(12)
Compound	Atom	U11	U22	U33	U12	U13	U23
$KBaEu(WO_4)_3$	Eu	0.0096(4)	0.0066(3)	0.0050(5)	0	0.0014(3)	0
	W1	0.0090(2)	0.0093(3)	0.0055(3)	-0.00101(12)	-0.00062(18)	0.00074(13)
	W2	0.0112(3)	0.0101(3)	0.0062(4)	0	0.0029(2)	0
	K	0.0114(5)	0.0110(5)	0.0145(7)	0.0014(3)	0.0033(4)	-0.0008(3)
	Ba	0.0114(5)	0.0110(5)	0.0145(7)	0.0014(3)	0.0033(4)	-0.0008(3)
	O1	0.012(3)	0.006(3)	0.013(3)	-0.004(2)	-0.001(2)	-0.001(3)
	O2	0.016(3)	0.024(3)	0.014(4)	-0.007(3)	-0.001(3)	0.003(3)
	O3	0.016(3)	0.009(3)	0.016(4)	-0.005(2)	0.006(3)	-0.006(3)
	O4	0.010(3)	0.019(3)	0.014(4)	-0.002(2)	0.000(2)	-0.002(3)
	O5	0.020(3)	0.018(3)	0.016(4)	0.004(3)	0.001(3)	0.001(3)

Table S5. The chromaticity coordinates of $KBaEu(XO_4)_3$ (X = Mo, W) at various temperature under excitation of 394 nm.

Temperature (K)	$KBaEu(MoO_4)_3$		$KBaEu(WO_4)_3$	
	CIE		CIE	
	x	y	x	y
300	0.668	0.330	0.666	0.333
325	0.669	0.331	0.666	0.333
350	0.669	0.331	0.666	0.333
375	0.668	0.331	0.666	0.334
400	0.667	0.332	0.666	0.334
425	0.667	0.332	0.665	0.335
450	0.667	0.332	0.665	0.335
475	0.667	0.333	0.664	0.335
500	0.666	0.334	0.664	0.336
525	0.666	0.334	0.663	0.336
550	0.665	0.334	0.663	0.336

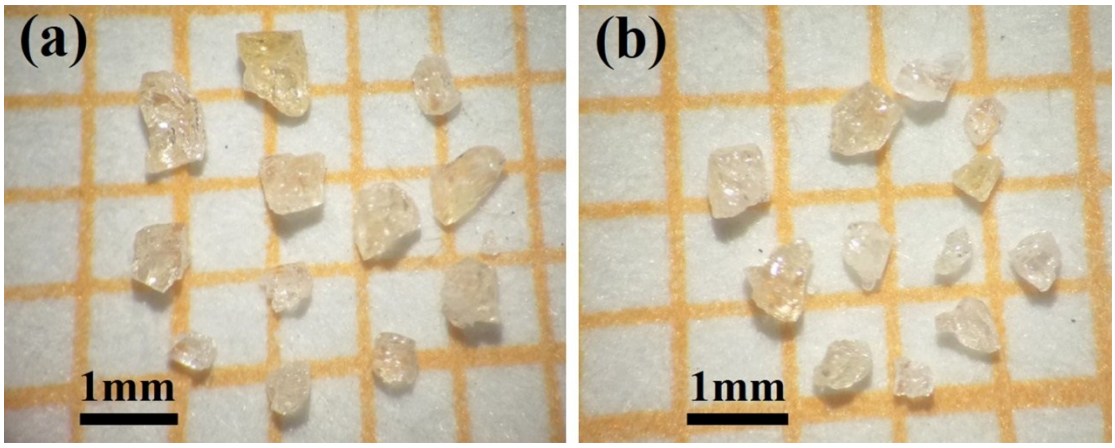


Figure S1. Photo of the as-synthesized $KBaEu(MoO_4)_3$ (a) and $KBaEu(WO_4)_3$ (b) crystals.

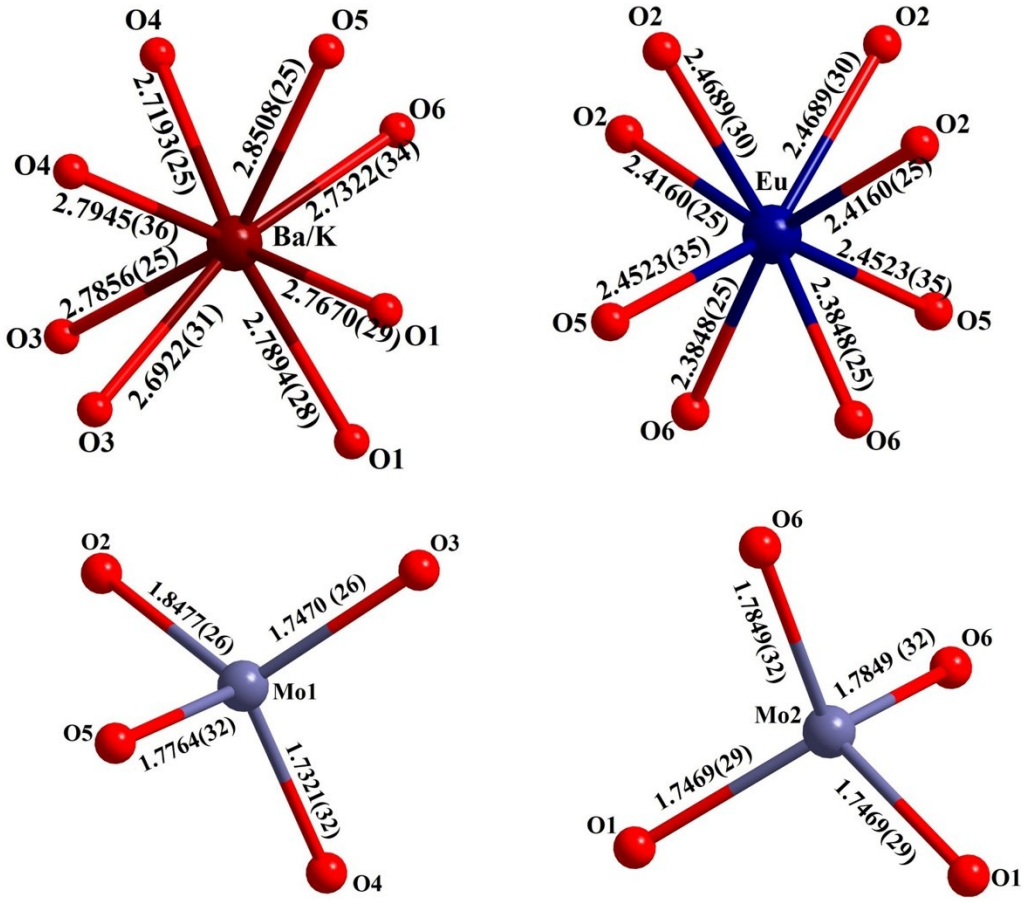


Figure S2. Coordination environments for Ba/K, Eu and Mo atoms in the structure of $KBaEu(MoO_4)_3$.

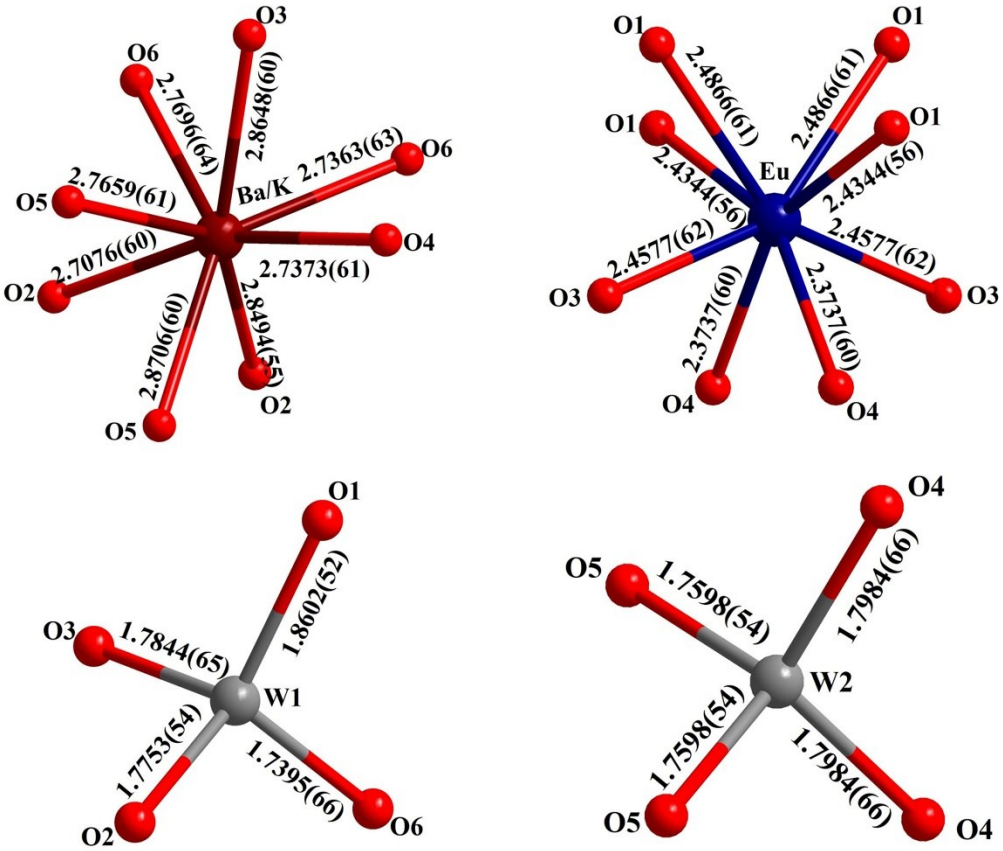
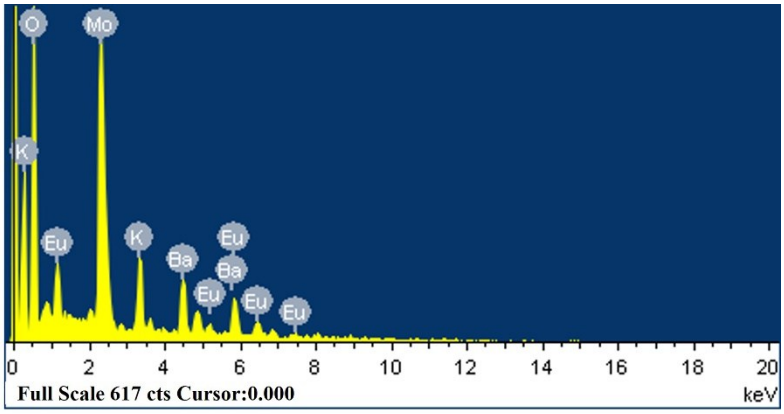
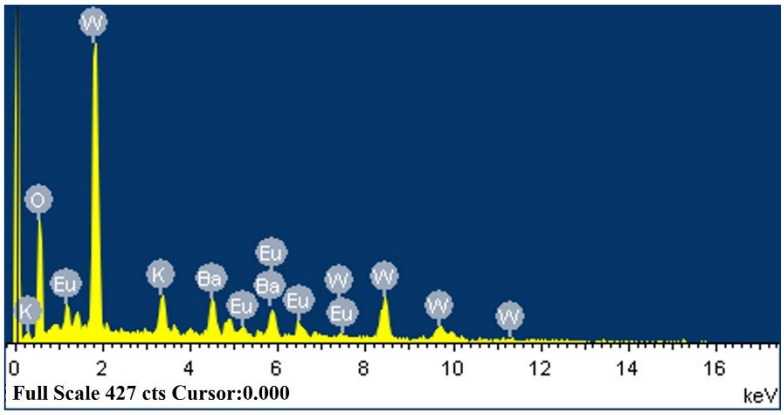


Figure S3. Coordination environments for Ba/K, Eu and W atoms in the structure of $KBaEu(WO_4)_3$.



(a)



(b)

Figure S4. EDX spectrum of $KBaEu(MoO_4)_3$ (a) and $KBaEu(WO_4)_3$ (b).

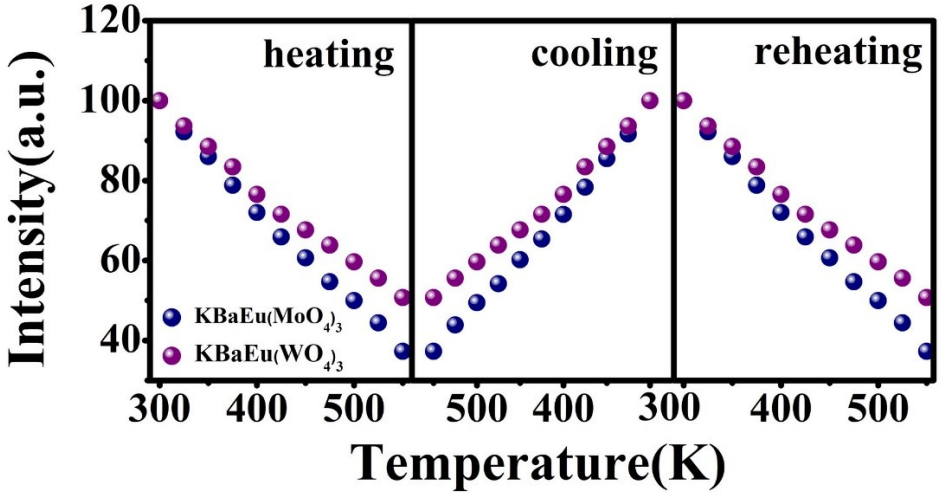


Figure S5. Plots of photoluminescence intensity versus temperature measured in the heating, cooling, and reheating processes (temperature-recycle measurements).