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Tb^{3+} and Yb^{3+} Doped Novel $KBaLu(MoO_4)_3$ Crystals with a Disorder Chained Structure Showing Dual-mode Luminescence Under UV or NIR Excitation

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

Atom	Wyck.	Site	x	y	z	U_{eq}[Å^2][a]
Lu	4e	2	0	0.11529(2)	3/4	0.0007(1)
K	8f	1	0.16413(3)	0.37451(4)	-0.07521(9)	0.0010(1)
Ba	8f	1	0.16413(3)	0.37451(4)	-0.07521(9)	0.0010(1)
Mo1	8f	1	0.15494(3)	0.10695(3)	1.39774(8)	0.0008(1)
Mo2	4e	2	0	0.34480(5)	1/4	0.0009(1)
O1	8f	1	0.0791(2)	0.4292(3)	0.4205(7)	0.0019(1)
O2	8f	1	-0.03929(19)	0.2648(3)	0.4737(7)	0.0014(1)
O3	8f	1	0.07416(18)	0.0371(3)	1.1422(6)	0.0011(1)
O4	8f	1	0.20574(19)	0.1976(3)	1.2466(7)	0.0015(1)
O5	8f	1	0.22780(19)	0.0284(3)	1.6191(7)	0.0016(1)
O6	8f	1	0.10877(18)	0.1845(3)	0.6048(6)	0.0013(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 $KBaLu(MoO_4)_3$.

Atoms	d(Å)	Atoms	d(Å)	Atoms	d(Å)
Lu—O6	2.367(3)	Mo1—O4	1.727(3)	K|Ba—O4iv	2.781(3)
Lu—O6i	2.367(3)	Mo1—O5	1.756(3)	K|Ba—O1v	2.748(3)
Lu—O2i	2.311(3)	Mo1—O6vii	1.779(3)	K|Ba—O6v	2.866(3)
Lu—O2	2.311(3)	Mo1—O3	1.868(3)	K|Ba—O4v	2.709(3)
Lu—O3	2.322(3)	Mo2—O1	1.757(3)	K|Ba—O2i	2.711(3)
Lu—O3i	2.322(3)	Mo2—O1viii	1.757(3)	K|Ba—O1vi	2.800(3)
Lu—O3ii	2.404(3)	Mo2—O2viii	1.789(3)	K|Ba—O5ix	2.874(3)
Lu—O3iii	2.404(3)	Mo2—O2	1.789(3)	K|Ba—O5x	2.699(3)

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

Table S3. Selected Bond Angles (deg) for $KBaLu(MoO_4)_3$.

Atoms	angles [deg]	Atoms	angles [deg]
O2i -Lu1-O2	76.40(17)	O6i-Lu1-O3ii	150.46(11)
O2i -Lu1-O3i	151.59(12)	O2i-Lu1-O3iii	123.07(11)
O2-Lu1-O3i	76.31(12)	O2-Lu1-O3iii	131.62(11)
O2i-Lu1-O3	76.31(12)	O3i-Lu1-O3iii	71.76(7)
O2-Lu1-O3	151.59(12)	O3-Lu1-O3iii	71.54(12)
O3i-Lu1-O3	131.72(16)	O6-Lu1-O3iii	150.46(11)
O2i-Lu1-O6	78.08(11)	O6i-Lu1-O3iii	71.16(11)
O2-Lu1-O6	69.39(11)	O3ii-Lu1-O3iii	79.33(15)
O3i-Lu1-O6	99.42(11)	O4-Mo1-O5	106.49(16)
O3-Lu1-O6	97.29(11)	O4-Mo1-O6iv	107.92(15)
O2i-Lu1-O6i	69.39(11)	O5-Mo1-O6iv	104.24(15)
O2-Lu1-O6i	78.08(11)	O4-Mo1-O3	109.74(15)
O3i-Lu1-O6i	97.29(11)	O5-Mo1-O3	120.07(15)
O3-Lu1-O6i	99.42(11)	O6 iv -Mo1-O3	107.75(14)
O6-Lu1-O6i	138.37(16)	O1-Mo2-O1v	108.60(2)
O2i-Lu1-O3ii	131.62(11)	O1-Mo2-O2v	105.63(16)
O2-Lu1-O3ii	123.07(11)	O v -Mo2-O2v	111.37(16)
O3i-Lu1-O3ii	71.54(12)	O1-Mo2-O2	111.37(16)
O3-Lu1-O3ii	71.76(7)	O1v -Mo2-O2	105.63(16)
O6-Lu1-O3ii	71.16(11)	O2v -Mo2-O2	114.20(2)

Symmetry codes: (i) -x,y,-z+3/2; (ii) x,-y,z-1/2; (iii) -x,-y,-z+2; (iv) x,y,z+1; (v) -x,y,-z+1/2;

Table S4. Anisotropic displacement parameters ($Å^2$) for $KBaLu(MoO_4)_3$.

Atom	U11	U22	U33	U12	U13	U23
Lu	0.0080(1)	0.0080(1)	0.0070(1)	0	0.0020(1)	0
Ba	0.0080(1)	0.0090(1)	0.01301)	0.0020(1)	0.0030(1)	-0.0010(1)
K	0.0080(1)	0.0090(1)	0.01301)	0.0020(1)	0.0030(1)	-0.0010(1)
Mo1	0.0070(1)	0.0090(1)	0.0070(1)	-0.0010(1)	0.0010(1)	0.0010(1)
Mo2	0.0100(1)	0.0090(1)	0.0080(1)	0	0.0040(1)	0
O1	0.0220(2)	0.0150(2)	0.0180(2)	-0.0020(2)	0.0040(1)	-0.0050(1)
O2	0.0130(2)	0.0170(2)	0.0150(2)	0.0040(1)	0.0080(1)	0.0020 (1)
O3	0.0110(2)	0.0110(2)	0.0110(2)	0.0020(1)	0.0020(1)	-0.0020(1)
O4	0.0140(2)	0.0150(2)	0.0170(2)	-0.0020(1)	0.0040(1)	0
O5	0.0170(2)	0.0180(2)	0.0130(2)	0.0010(1)	0.0050(1)	0.0070(1)
O6	0.0120(2)	0.0120(2)	0.0170(2)	-0.0010(1)	0.0060(1)	0

Table S5. Raman wavenumbers (cm^{-1}) for $KBaLu(MoO_4)_3$.

78.90	325.85
113.99	338.06
130.11 w	378.28
135.40 w	417.75
153.04	735.04
162.63	836.46
173.31	874.28
183.53	900.98
219.60 w	925.12
285.82	943.56

w – weak line.

Table S6. The chromaticity coordinates of Tb^{3+} and Tb^{3+}/Yb^{3+} doped $KBaLu(MoO_4)_3$ at room temperature under various excitations.

Excitations (nm)	Tb^{3+}: KBLM		Tb^{3+}/Yb^{3+}: KBLM	
	CIE		CIE	
	x	y	x	y
275	0.326	0.616	0.324	0.618
365	0.294	0.411	0.299	0.410
485	0.364	0.628	0.359	0.633
980	—	—	0.315	0.611

Table S7. The chromaticity coordinates of $KBaLu(MoO_4)_3$: Tb^{3+}, Yb^{3+} at various temperature under excitation of 275 nm.

Temperature (K)	KBLM: Tb^{3+}, Yb^{3+}	
	CIE	
	x	y
300	0.326	0.616
325	0.327	0.609
350	0.326	0.604
375	0.325	0.596
400	0.326	0.589
425	0.326	0.580
450	0.327	0.569
475	0.327	0.560
500	0.327	0.551
525	0.326	0.541
550	0.327	0.530

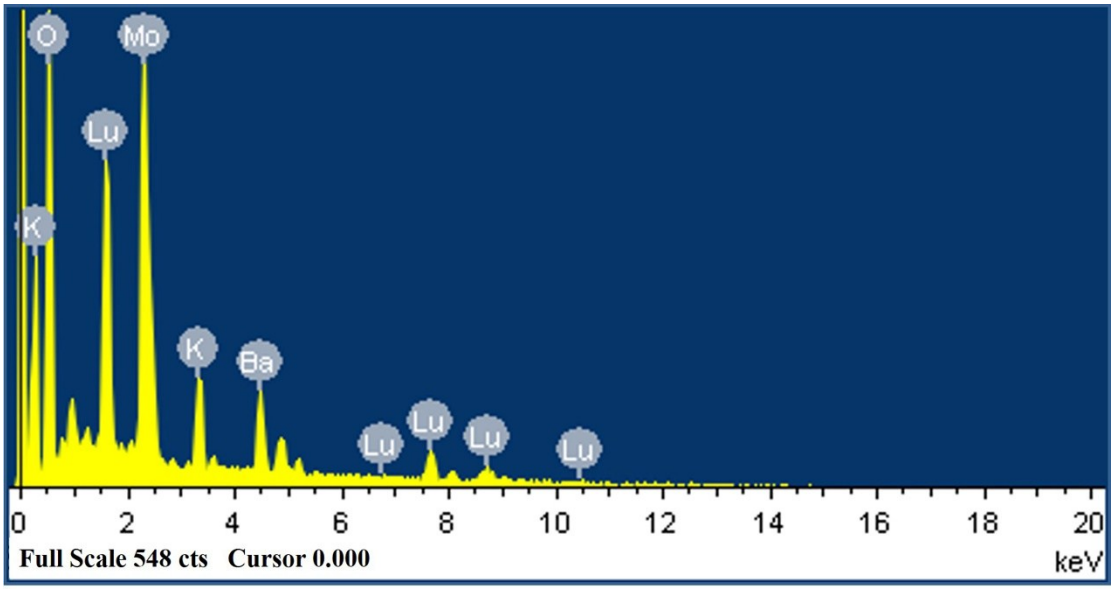

Fig. S1. EDX spectrum of $KBaLu(MoO_4)_3$ crystal.

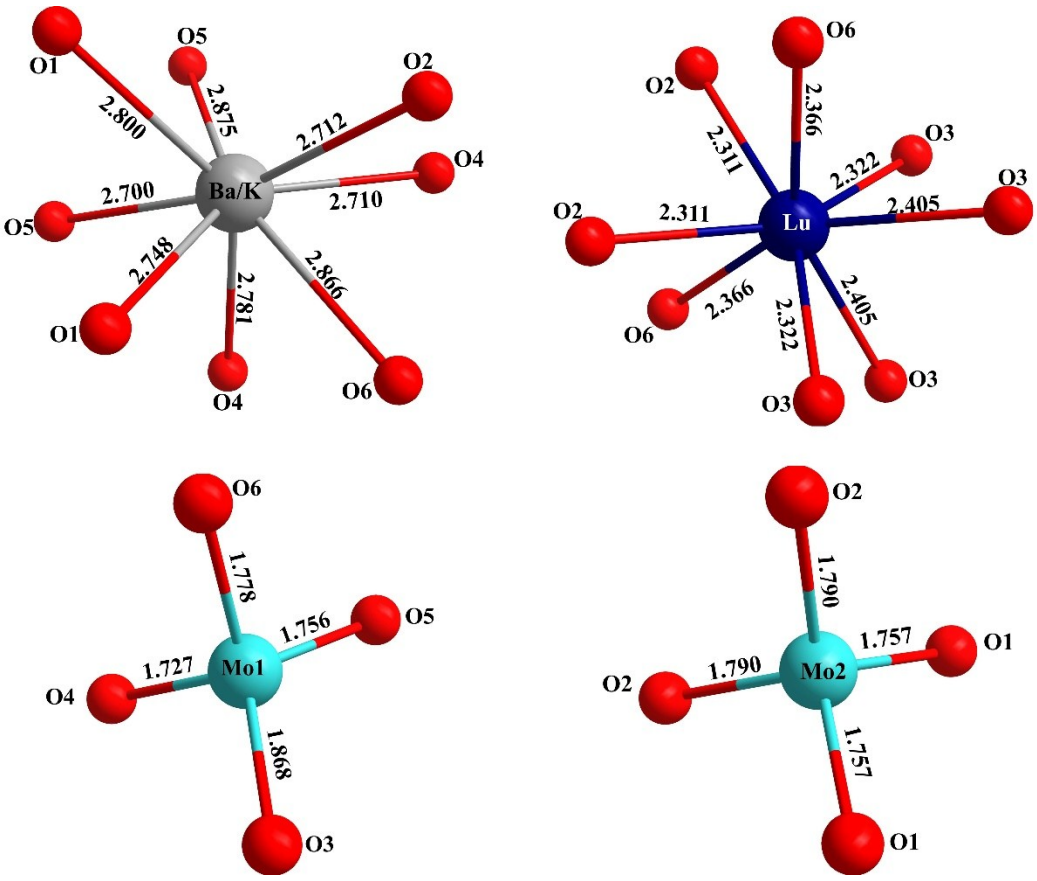

Fig. S2. Coordination environments for Ba/K, Lu and Mo atoms in the structure of $KBaLu(MoO_4)_3$.

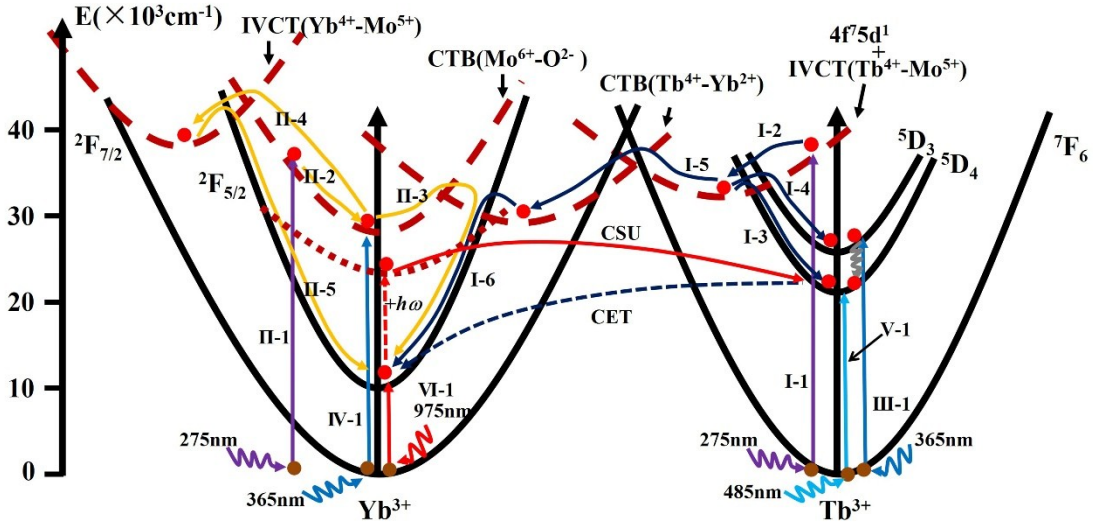

Fig. S3. A schematic configurational coordinate diagram of Tb^{3+} and Yb^{3+} ions in $KBaLu(MoO_4)_3$.

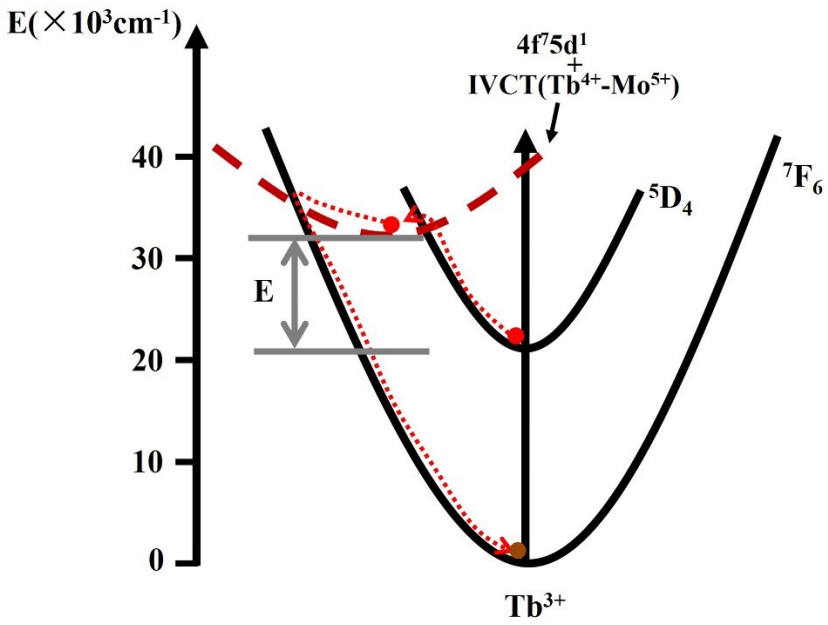

Fig. S4. Plot of pathways for the thermal quenching of the $^5D_4$ state of Tb^{3+} through a IVCT band.

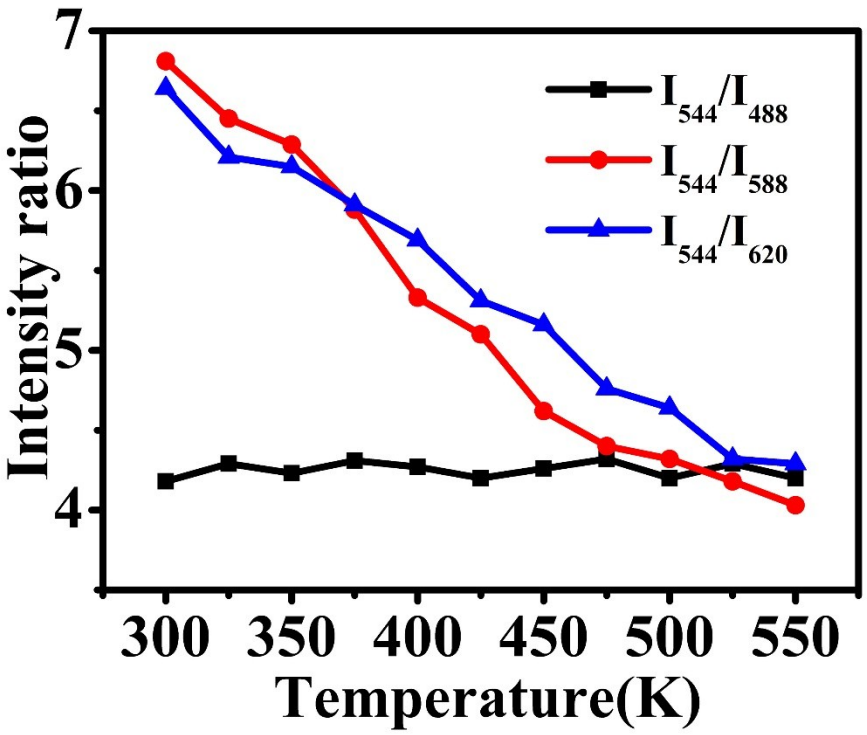

Fig. S5. The ratio of the integrated intensity of $^5D_4 \rightarrow {}^7F_5/{}^5D_4 \rightarrow {}^7F_6$ transitions, $^5D_4 \rightarrow {}^7F_5/{}^5D_4 \rightarrow {}^7F_4$ and $^5D_4 \rightarrow {}^7F_5/{}^5D_4 \rightarrow {}^7F_3$ transitions as temperature rise from 300K to 550K.