

Supplementary Information for

“Influence of annealing conditions on the structure and luminescent properties of $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ ($0 \leq x \leq 1$)”

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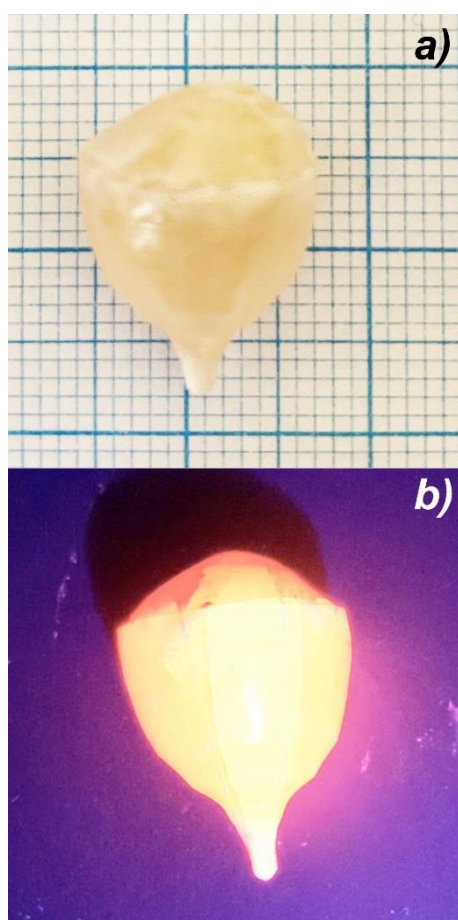


Figure S1. The photos of the $\text{KGd}_{0.8}\text{Eu}_{0.2}(\text{MoO}_4)_2$ crystal grown by Czochralski technique under the daily light (a) and under the excitation (~ 395 nm) (b).

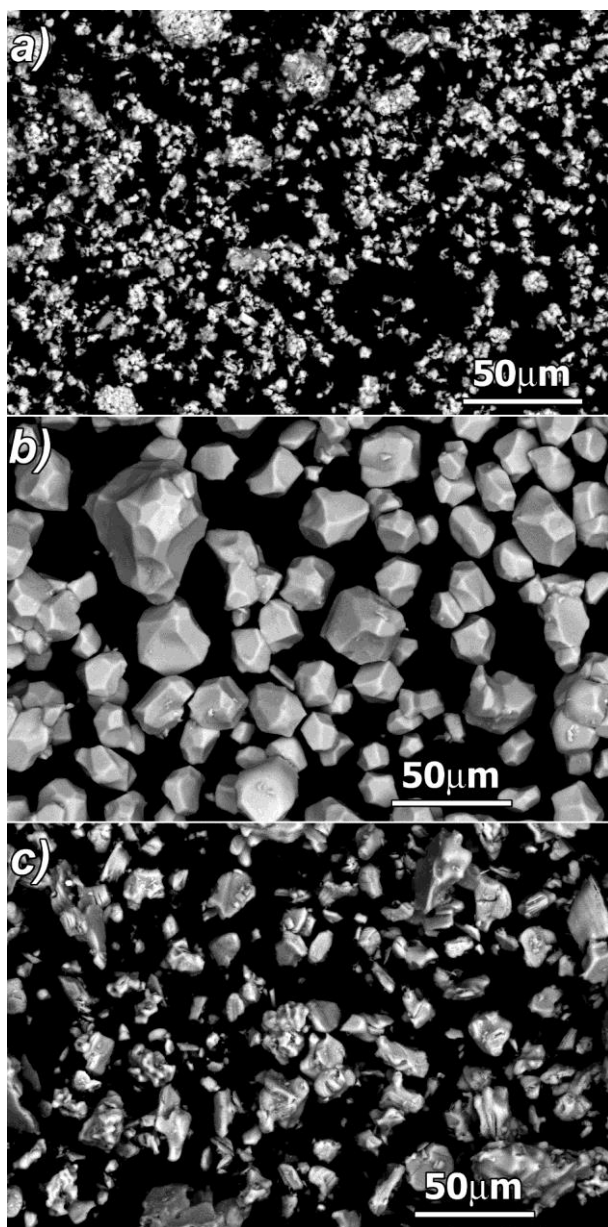


Figure S2. SEM images of $\text{KEu}(\text{MoO}_4)_2$ prepared at 923 K (a) and $\text{KR}(\text{MoO}_4)_2$ ($R = \text{Eu}$ (b), Gd (c)) prepared at 1223 K.

Table S1. EDX analysis results of $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ ($x = 0.2, 0.4, 0.5$)

	$\text{KGd}_{0.8}\text{Eu}_{0.2}(\text{MoO}_4)_2$	$\text{KGd}_{0.6}\text{Eu}_{0.4}(\text{MoO}_4)_2$	$\text{KGd}_{0.5}\text{Eu}_{0.5}(\text{MoO}_4)_2$
Sample preparation	crystal grown by the CZ technique	ceramic technique at 1223 K	
K, at. %	25.71±0.92	25.54±2.50	25.71±1.75
Mo, at. %	52.59±1.09	54.86±2.39	53.43±3.24
Gd, at. %	17.79±1.20	12.00±2.95	10.62±2.54
Eu, at. %	3.91±0.42	7.61±1.82	10.24±2.37
Gd:Eu ratio	0.82(1):0.18(1)	0.61(1):0.39(1)	0.51(2):0.49(2)

Table S2. Unit cell parameters for $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ ($0 \leq x \leq 1$) solid solutions prepared by heating at 923 K as determined from PXRD patterns (SG $P\bar{1}$, $Z = 2$).

x	a , Å	b , Å	c , Å	α , deg.	β , deg.	γ , deg.	V/Z , Å ³
0	11.1830(2)	5.2820(1)	6.9105(1)	112.413(2)	111.545(2)	91.086(2)	172.47
0.10	11.1857(2)	5.2844(1)	6.9132(1)	112.423(2)	111.553(1)	91.074(2)	172.64
0.20	11.1841(3)	5.2857(2)	6.9157(2)	112.428(2)	111.561(2)	91.065(2)	172.71
0.25	11.1887(3)	5.2898(1)	6.9206(1)	112.431(2)	111.563(1)	91.062(2)	173.03
0.30	11.1845(2)	5.2869(1)	6.9177(1)	112.429(2)	111.565(1)	91.059(2)	172.80
0.40	11.1823(3)	5.2877(1)	6.9198(1)	112.435(2)	111.566(2)	91.058(2)	172.84
0.50	11.1802(2)	5.2888(1)	6.9212(1)	112.442(2)	111.574(1)	91.047(2)	172.86
0.60	11.1808(3)	5.2901(1)	6.9243(2)	112.441(2)	111.577(2)	91.035(2)	172.99
0.70	11.1824(4)	5.2931(2)	6.9279(2)	112.446(2)	111.585(2)	91.033(2)	173.19
0.80	11.1797(2)	5.2940(1)	6.9291(1)	112.451(1)	111.594(1)	91.027(1)	173.19
0.90	11.1831(4)	5.2966(2)	6.9318(2)	112.449(2)	111.600(2)	91.021(2)	173.39
1	11.1784(4)	5.2961(2)	6.9326(2)	112.459(2)	111.603(2)	91.005(2)	173.31

Table S3. Unit cell parameters for $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ ($0 \leq x \leq 1$) prepared at 1073 K as determined from PXRD patterns.

x	a , Å	b , Å	c , Å	α , deg.	β , deg.	γ , deg.	V/Z , Å ³
0 ¹	11.1812(2)	5.2812(1)	6.9093(1)	112.420(1)	111.546(1)	91.080(2)	172.38
0.10	11.1837(3)	5.2842(2)	6.9128(2)	112.456(3)	111.564(2)	91.048(3)	172.54
0.20	11.1797(3)	5.2845(2)	6.9137(2)	112.440(2)	111.559(2)	91.060(2)	172.54
0.30	11.1816(3)	5.2873(2)	6.9178(2)	112.438(2)	111.569(2)	91.049(2)	172.76
0.40	11.1809(3)	5.2888(1)	6.9199(2)	112.435(2)	111.566(1)	91.061(2)	172.85
0.50	11.1774(2)	5.2901(1)	6.9221(1)	112.446(2)	111.572(1)	91.047(2)	172.88
0.60	11.1756(3)	5.2863(2)	6.9200(2)	112.438(2)	111.573(2)	91.040(2)	172.69
0.70	11.1795(3)	5.2943(2)	6.9275(2)	112.454(2)	111.584(2)	91.036(2)	173.16
0.80	11.1775(2)	5.2947(2)	6.9290(1)	112.456(2)	111.596(2)	91.018(2)	173.17
0.90	11.1804(4)	5.2951(2)	6.9291(2)	112.457(3)	111.589(2)	91.020(3)	173.24
	5.5295(1)	5.2769(1)	11.7269(3)			91.246(2)	171.05
1 ²	5.5295(2)	5.2767(2)	11.7094(5)			91.219(2)	170.79

¹ anorthic α -phase (SG $P\bar{1}$, $Z = 2$)

² β -phase with the incommensurate modulated structure (SSG $I2/b(\alpha\beta 0)00$, $Z = 2$)

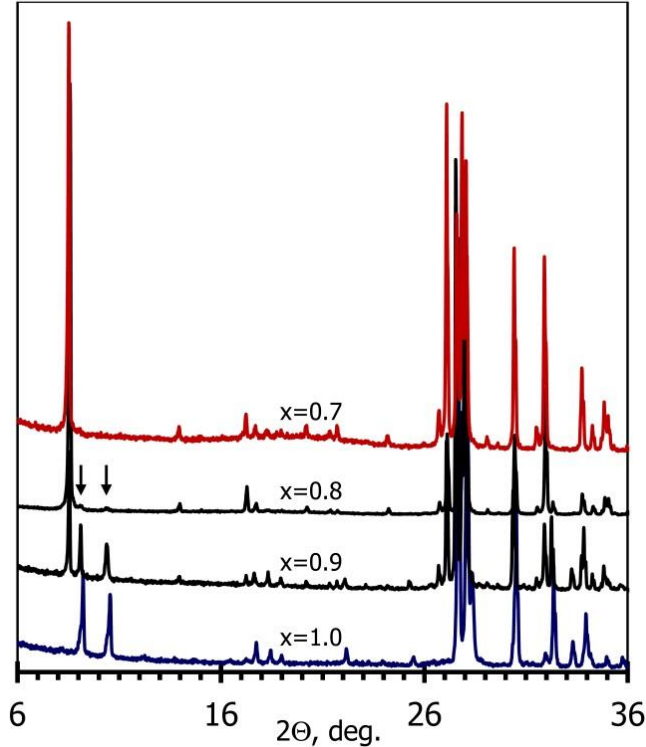


Figure S3. Parts of PXRD patterns of $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ ($0.7 \leq x \leq 1$) annealed at 1073 K. The small intensity reflections of the monoclinic β -phase in $\text{KGd}_{0.2}\text{Eu}_{0.8}(\text{MoO}_4)_2$ are marked with arrows.

Table S4. Unit cell parameters for $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ ($0 \leq x \leq 1$, main phases) prepared at 1173 K as determined from PXRD patterns.

x	a , Å	b , Å	c , Å	α , deg.	β , deg.	γ , deg.	V/Z , Å ³
0	5.1165(3)	18.0775(4)	8.0384(9)				185.88
0.10	5.1160(2)	18.0759(5)	8.0479(5)				186.06
0.20	5.1218(4)	18.0713(5)	8.0522(6)				186.32
0.30	5.1295(4)	18.0759(6)	8.0566(5)				186.76
x	a , Å	b , Å	c , Å	q		γ , deg.	V/Z , Å ³
0.40	5.5196(1)	5.2724(1)	11.7122(4)	0.5659(1) a^* -0.1203(2) b^*		91.239(2)	170.38
0.50	5.5163(2)	5.2702(2)	11.7010(3)	0.5638(2) a^* -0.1194(3) b^*		91.258(3)	170.05
0.60	5.5134(2)	5.2720(1)	11.7053(3)	0.5656(1) a^* -0.1185(2) b^*		91.264(3)	170.08
0.70	5.5047(2)	5.2728(2)	11.6935(5)	0.5669(3) a^* -0.1214(3) b^*		91.216(3)	169.66
0.80	5.4946(6)	5.2798(4)	11.7002(9)	0.5671(3) a^* -0.1202(5) b^*		91.325(7)	169.67
0.90	5.5252(3)	5.2792(3)	11.7226(6)	0.5678(3) a^* -0.1207(4) b^*		91.231(3)	170.93
1	5.5238(3)	5.2812(2)	11.7217(5)	0.5712(3) a^* -0.1177(3) b^*		91.270(3)	170.93

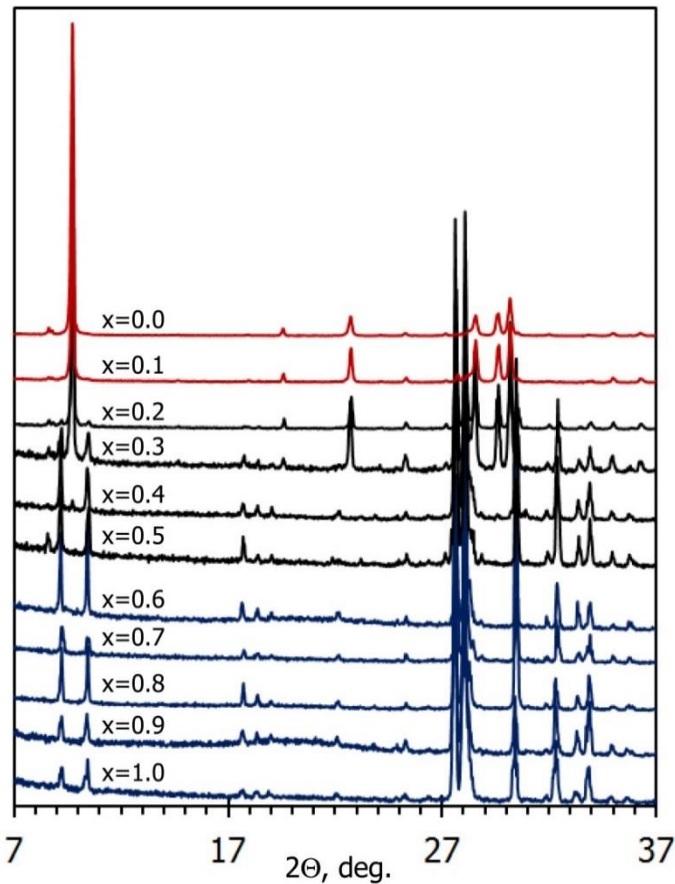


Figure S4. Parts of PXRD patterns of $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ annealed at 1173 K.

Table S5. Unit cell parameters for $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ ($0 \leq x \leq 1$, main phases) prepared at 1223 K as determined from PXRD patterns.

x	a , Å	b , Å	c , Å	α , deg.	β , deg.	γ , deg.	V , Å ³
0	5.1163(2)	18.0772(4)	8.0413(5)				185.93
0.10	5.1151(2)	18.0728(4)	8.0462(5)				185.96
0.20	5.1187(3)	18.0681(5)	8.0504(6)				186.14
0.30	5.1181(3)	18.0600(7)	8.0573(6)				186.19
0.40	5.1102(3)	18.0794(6)	8.0661(1)				186.30
	11.206(2)	5.284(1)	6.920(1)	112.33(1)	111.61(2)	91.08(1)	173.16
0.50	5.2059(2)	18.0501(3)	8.0568(3)				186.08
	11.206(2)	5.284(1)	6.920(1)	112.33(1)	111.61(2)	91.08(1)	173.16
0.60	11.1771(2)	5.2907(1)	6.9209(2)	112.396(3)	111.599(2)	91.073(2)	172.88
0.70	11.1805(6)	5.2956(2)	6.9293(2)	112.444(4)	111.571(4)	91.011(4)	173.31
x	a , Å	b , Å	c , Å	$\mathbf{q}$		γ , deg.	V , Å ³
0.80	5.5208(3)	5.2775(3)	11.7036(6)	0.5684(3) $\mathbf{a}^*$ -0.1236(5) $\mathbf{b}^*$		91.230(3)	170.46
0.90	5.5246(5)	5.2795(4)	11.717(1)	0.5683(2) $\mathbf{a}^*$ -0.1243(5) $\mathbf{b}^*$		91.249(2)	170.84
1	5.5274(1)	5.2801(1)	11.7150(2)	0.5672(1) $\mathbf{a}^*$ -0.1260(2) $\mathbf{b}^*$		91.222(1)	170.91

Table S6. Fractional atomic coordinates, site symmetry, isotropic displacement atomic parameters (U_{iso}) and site occupation for $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ ($x = 0, 0.2$).

Atom	x	x	y	z	$U_{\text{iso}}*100$
R	0	0	0.0073(1)	$\frac{1}{4}$	2.45(6)
	0.2*	0	0.0049(2)	$\frac{1}{4}$	1.91(7)
K	0	$\frac{1}{2}$	0.2702(3)	$\frac{1}{4}$	2.65(17)
	0.2	$\frac{1}{2}$	0.2698(5)	$\frac{1}{4}$	0.13(15)
Mo	0	0.5184(3)	0.10260(8)	0.9839(2)	2.49(6)
	0.2	0.5195(3)	0.1034(1)	0.9835(2)	0.85(6)
O1	0	0.721(1)	0.0959(8)	0.1516(9)	0.67(13)
	0.2	0.732(2)	0.096(1)	0.1521(9)	0.17(15)
O2	0	0.741(1)	0.0968(7)	0.7963(10)	0.67(13)
	0.2	0.728(1)	0.085(1)	0.7832(11)	0.17(15)
O3	0	0.246(1)	0.0360(5)	-0.0164(14)	0.67(13)
	0.2	0.233(1)	0.0361(9)	0.001(2)	0.17(15)
O4	0	0.340(1)	0.1962(6)	-0.0331(9)	0.67(13)
	0.2	0.382(1)	0.196(1)	-0.016(1)	0.17(15)

* $R = 0.8\text{Gd}^{3+} + 0.2\text{Eu}^{3+}$

Table S7. Selected distances ($\text{\AA}$) in $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ ($x = 0, 0.2$).

Polyhedra	Distance, $\text{\AA}$	$x=0$	$x=0.2$
RO_8	$R\text{-O1}\times 2$	2.29(1)	2.29(2)
	$R\text{-O2}\times 2$	2.33(1)	2.16(2)
	$R\text{-O3}\times 2$	2.54(1)	2.40(2)
	$R\text{-O3}\times 2$	2.39(1)	2.46(2)
	$\langle R\text{-O} \rangle$	2.39	2.33
KO_8	$\text{K-O1}\times 2$	3.442(15)	3.45(2)
	$\text{K-O2}\times 2$	2.772(13)	2.98(2)
	$\text{K-O4}\times 2$	2.701(9)	2.59(2)
	$\text{K-O4}\times 2$	2.718(7)	2.78(2)
	$\langle \text{K-O} \rangle$	2.91	2.95
MoO_4	Mo-O1	1.704(7)	1.745(8)
	Mo-O2	1.892(7)	1.960(9)
	Mo-O3	1.843(8)	1.910(12)
	Mo-O4	1.822(11)	1.820(2)
	$\langle \text{Mo-O} \rangle$	1.82	1.86

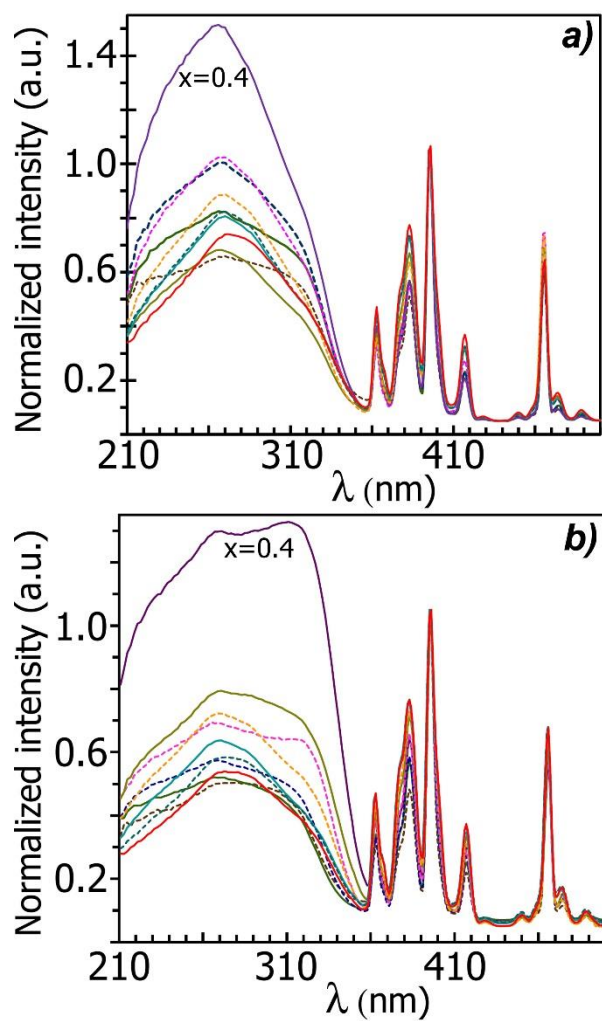


Figure S5. PLE ($\lambda_{\text{em}} = 610\text{-}625$ nm) spectra at room temperature of $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ ($0.1 \leq x \leq 1$) prepared at 1173 K (a) and 1223 K (b). PLE spectra are normalized to the peak of the excitation of the ${}^7\text{F}_0 \rightarrow {}^5\text{L}_6$ transition (395 nm).

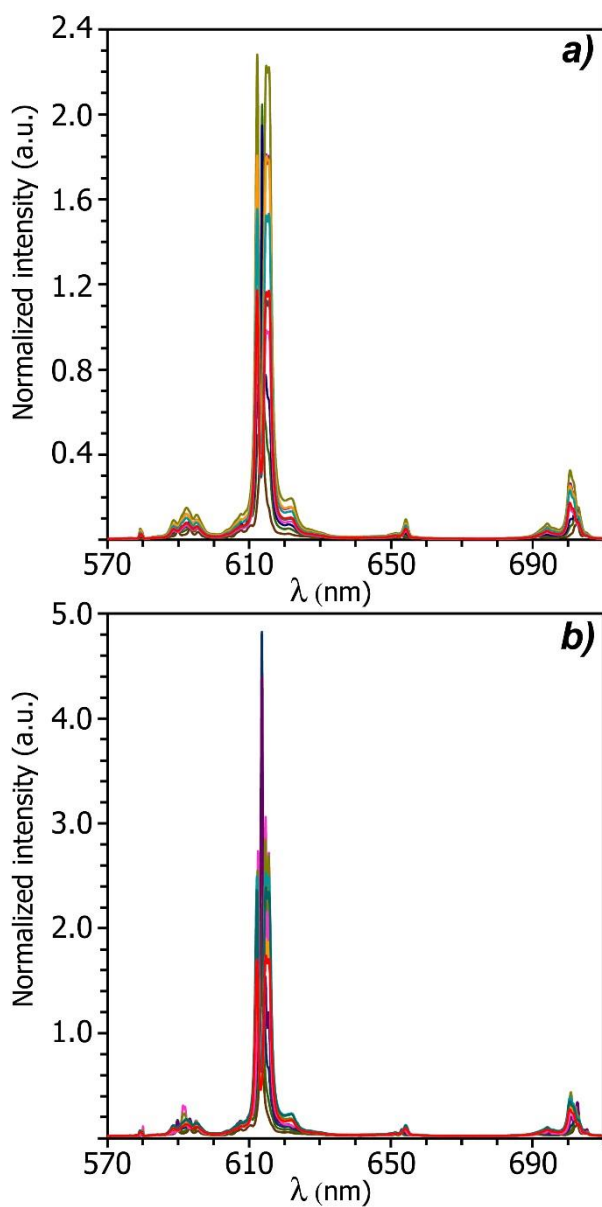


Figure S6. PL ($\lambda_{\text{ex}} = 395$ nm) spectra at room temperature of $\text{KGd}_{1-x}\text{Eu}_x(\text{MoO}_4)_2$ ($0.1 \leq x \leq 1$) prepared at 1173 K (a) and 1223 K (b). All PL spectra are normalized on the intensity value of $\alpha\text{-KEu}(\text{MoO}_4)_2$.