Supplementary Information

$KLn(MoO_4)_2$ micro/nanocrystals (Ln = La-Lu, Y): systematic hydrothermal crystallization, structure, and the performance of doped Eu^{3+} for optical thermometry

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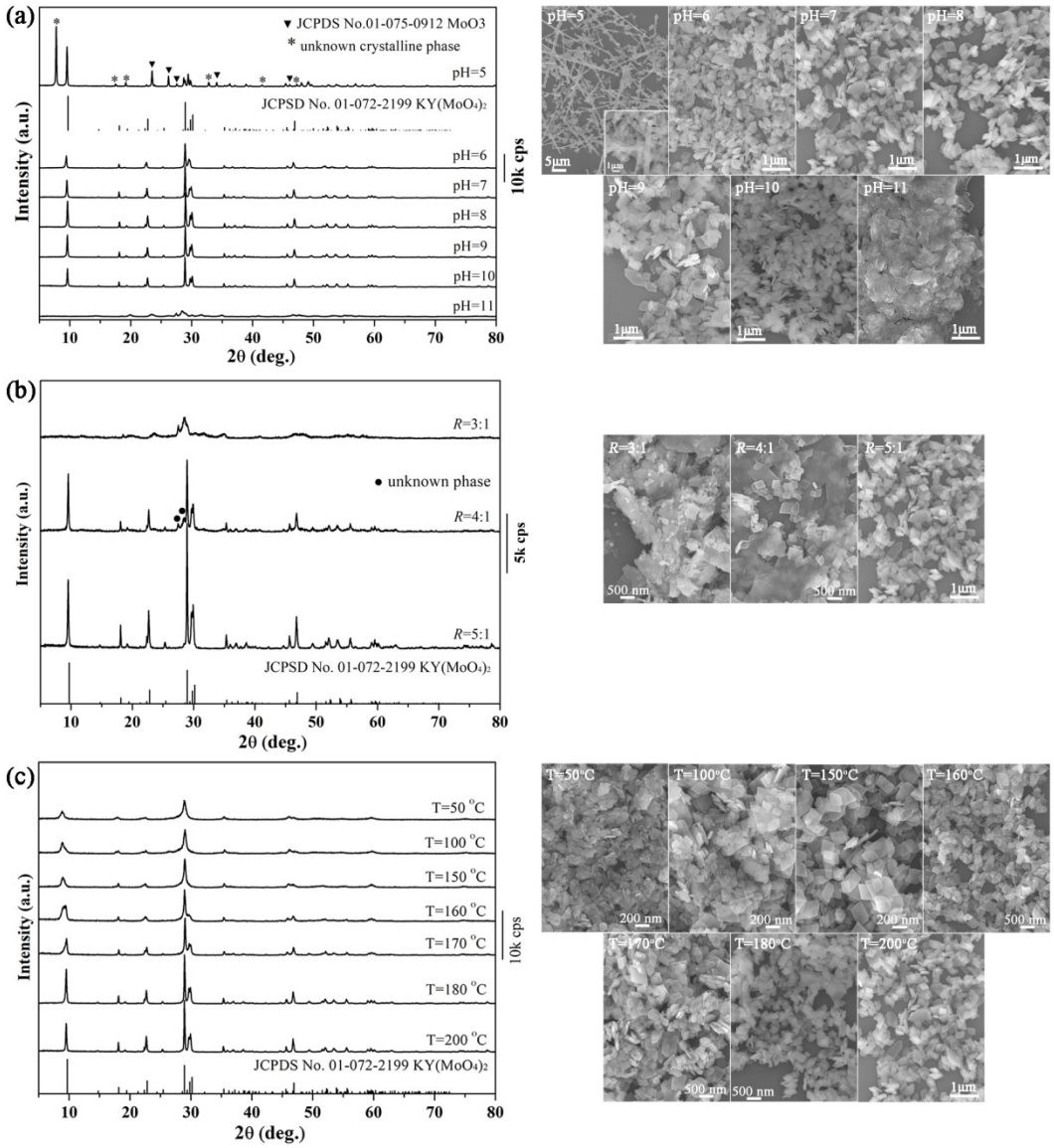

Fig. S1. XRD patterns (left part) and crystallite morphology (right part) for the Ln = Y samples prepared under (a) different pH values when R = 5 and T = 200 °C, (b) different R values when pH = 7 and T = 200 °C, and (c) different hydrothermal temperatures when pH = 7 and R = 5.

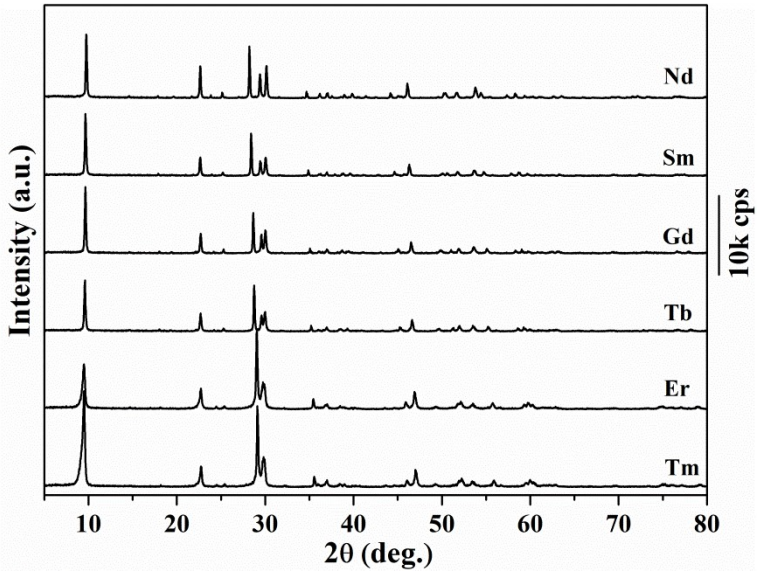

Fig. S2. XRD patterns of the hydrothermal products for Ln = Nd, Sm, Gd, Tb, Er and Tm.

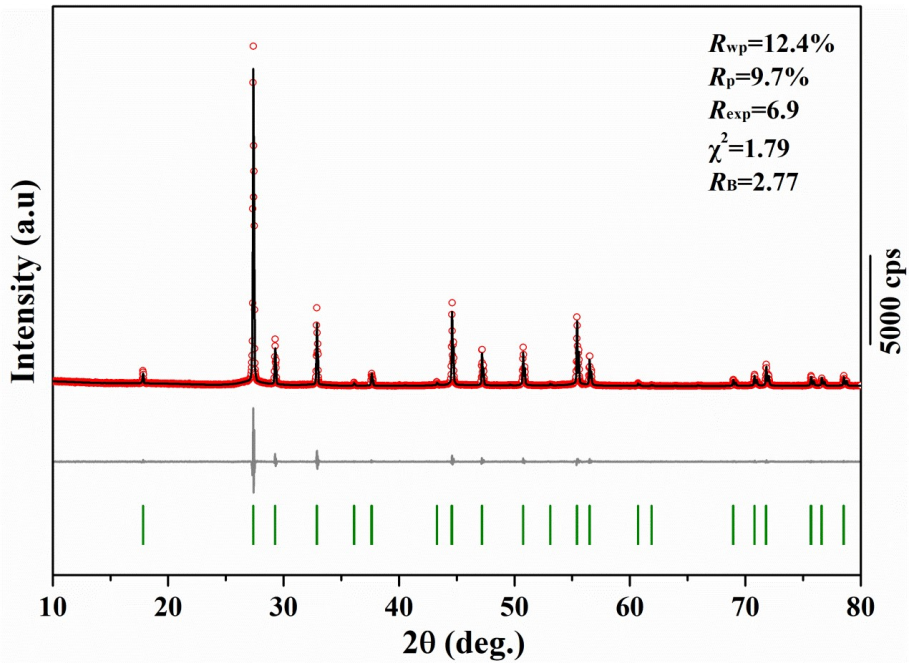

Fig. S3. Rietveld refinement of the XRD pattern for monoclinic $KLa(MoO_4)_2$.

Table S1. Fractional atomic coordinates (*x*, *y*, *z*) and main bond lengths (Å) for the orthorhombic structure of $KLa(MoO_4)_2$.

	Coordinates			Bond length			
	x	*y*	*z*				
K	0.25	0.636(2)	0	K-O1(×2)	2.653(4)	La-O1(×2)	2.565(3)
La	0.25	0.622(8)	0	K-O1(×2)	2.700(1)	La-O1(×2)	2.581(8)
Mo	0.25	0.125(8)	0	K-O2(×2)	2.502(3)	La-O2(×2)	2.573(1)
O1	0.010 (3)	0.040(7)	0.240(3)	K-O2(×2)	2.508(8)	La-O2(×2)	2.635(2)
O2	0.0069(3)	0.207(2)	-0.152(4)	Mo-O1	1.855(9)	Mo-O2	1.854(6)

Table S2. The 2Theta (°), *d*-spacing (Å) and Miller index (*h*, *k*, *l*) derived via Rietveld refinement of the XRD pattern for $KY(MoO_4)_2$.

No.	2Theta (°)	*d*-spacing (Å)	*h*	*k*	*l*
1	9.579	9.22545	0	2	0
2	14.704	6.01965	0	2	1
3	18.105	4.89571	1	1	0
4	19.226	4.61273	0	4	0
5	21.302	4.16777	1	1	1
6	22.365	3.97187	0	0	2
7	22.691	3.91565	1	3	0
8	24.379	3.64813	0	2	2
9	25.339	3.51215	1	3	1
10	28.431	3.13681	1	4	1
11	28.508	3.12847	1	0	2
12	28.924	3.08444	1	1	2
13	29.013	3.07515	0	6	0
14	29.657	3.00983	0	4	2
15	29.908	2.98514	1	5	0
16	32.003	2.79435	1	5	1
17	35.324	2.53886	2	0	0
18	35.936	2.49705	1	6	1
19	36.683	2.44785	2	2	0
20	36.938	2.43155	0	6	2
21	37.665	2.38631	1	5	2
22	38.626	2.32907	1	1	3
23	39.022	2.30636	0	8	0
24	39.198	2.29644	0	4	3
25	39.576	2.27532	1	2	3
26	40.029	2.25061	2	3	1
27	40.15	2.24413	1	7	1
28	40.525	2.22421	2	4	0
29	40.703	2.2149	0	8	1
30	41.119	2.19346	1	3	3
31	42.212	2.13917	2	0	2
32	43.202	2.0924	1	4	3
33	43.387	2.08389	2	2	2
34	44.596	2.03016	1	8	1
35	44.77	2.02269	2	5	1
36	45.438	1.99449	0	8	2
37	45.645	1.98594	0	0	4
38	46.752	1.94146	0	2	4
39	46.773	1.94064	2	4	2
40	47.81	1.90094	2	6	1
41	48.759	1.86613	1	6	3

42	49.031	1.85642	1	8	2
43	49.352	1.84509	0	10	0
44	50.751	1.79746	2	2	3
45	51.224	1.78197	2	7	1
46	51.559	1.77116	1	3	4
47	52.035	1.75608	2	6	2
48	52.029	1.75628	2	3	3
49	52.127	1.75319	1	7	3
50	52.58	1.73915	0	8	3
51	53.388	1.71472	1	9	2
52	53.644	1.70714	2	8	0
53	54.389	1.68549	3	1	0
54	54.997	1.66829	0	6	4
55	55.259	1.661	2	7	2
56	55.533	1.65346	1	5	4
57	55.704	1.64879	3	1	1
58	56.332	1.6319	3	3	0
59	57.617	1.59852	3	3	1
60	57.847	1.5927	1	11	0
61	57.984	1.58928	1	10	2
62	58.158	1.58494	1	6	4
63	58.591	1.57425	2	6	3
64	58.83	1.5684	2	8	2
65	58.942	1.5657	0	2	5
66	59.021	1.5638	2	9	1
67	59.003	1.56423	2	0	4
68	59.111	1.56163	1	11	1
69	59.235	1.55864	2	1	4
70	59.258	1.55811	3	4	1
71	59.301	1.55709	3	0	2
72	59.533	1.55157	3	1	2
73	59.844	1.54425	1	9	3
74	59.93	1.54222	2	2	4
75	60.13	1.53758	0	12	0
76	60.092	1.53846	3	5	0
77	60.225	1.53537	3	2	2
78	61.078	1.51597	2	3	4
79	61.174	1.51382	0	10	3
80	61.166	1.51399	1	7	4
81	61.293	1.51117	1	1	5
82	61.365	1.50956	0	12	1
83	61.327	1.5104	3	5	1
84	61.369	1.50946	3	3	2
85	61.575	1.50491	0	8	4

86	61.587	1.50466	2	7	3
87	61.701	1.50215	0	4	5
88	61.974	1.49619	1	2	5
89	62.141	1.49257	2	10	0
90	62.663	1.48137	2	4	4
91	62.722	1.48013	2	9	2
92	62.809	1.47828	1	11	2
93	62.95	1.4753	3	4	2
94	63.099	1.47218	1	3	5
95	63.353	1.4669	2	10	1
96	63.803	1.45763	3	6	1
97	64.143	1.45072	1	10	3
98	64.329	1.44697	1	12	1
99	64.534	1.44288	1	8	4
100	64.656	1.44044	1	4	5
101	64.669	1.44019	2	5	4
102	64.942	1.4348	2	8	3
103	64.988	1.43388	0	12	2
104	64.951	1.4346	3	5	2
105	65.484	1.42422	3	7	0
106	65.605	1.42188	3	1	3
107	66.149	1.4115	0	6	5
108	66.262	1.40938	3	2	3
109	66.629	1.40249	1	5	5
110	66.663	1.40187	3	7	1
111	66.916	1.39718	2	10	2
112	67.076	1.39422	2	6	4
113	67.354	1.38916	3	6	2
114	67.348	1.38926	3	3	3
115	67.865	1.37992	1	12	2
116	67.957	1.37828	2	11	1
117	68.24	1.37326	1	9	4
118	68.601	1.36691	1	13	0
119	68.637	1.36629	2	9	3
120	68.72	1.36483	1	11	3
121	68.855	1.36248	3	4	3
122	69.002	1.35994	1	6	5
123	69.481	1.35173	0	10	4
124	69.754	1.34711	1	13	1
125	69.868	1.34519	2	7	4
126	69.888	1.34485	3	8	1
127	69.986	1.34321	2	1	5
128	70.14	1.34064	3	7	2
129	70.622	1.33266	2	2	5

130	70.805	1.32966	0	12	3
131	70.77	1.33023	3	5	3
132	71.157	1.32396	0	0	6
133	71.405	1.31996	2	11	2
134	71.532	1.31792	0	14	0
135	71.704	1.31519	2	12	0
136	71.677	1.31561	2	3	5
137	71.759	1.31432	1	7	5
138	71.999	1.31053	0	2	6
139	72.136	1.30837	0	8	5
140	72.273	1.30624	1	10	4
141	72.338	1.30522	3	9	0
142	72.665	1.30015	0	14	1
143	72.659	1.30023	2	10	3
144	72.835	1.29753	2	12	1
145	73.028	1.29457	2	8	4
146	73.081	1.29376	3	6	3
147	73.164	1.29251	1	13	2
148	73.144	1.29281	2	4	5
149	73.295	1.29051	3	8	2
150	73.465	1.28795	3	9	1
151	73.449	1.28819	3	0	4
152	73.575	1.28629	1	12	3
153	73.658	1.28506	3	1	4
154	73.921	1.28113	1	0	6
155	74.129	1.27805	1	1	6
156	74.281	1.27581	3	2	4
157	74.502	1.27258	0	4	6
158	74.718	1.26943	4	0	0
159	74.751	1.26895	1	2	6
160	74.887	1.26698	1	8	5
161	75.013	1.26516	2	5	5
162	75.316	1.26083	3	3	4
163	75.408	1.25952	1	14	1
164	75.545	1.25758	4	2	0
165	75.777	1.2543	3	7	3
166	75.784	1.2542	1	3	6
167	76.022	1.25086	0	14	2
168	76.038	1.25064	4	1	1
169	76.19	1.24852	2	12	2
170	76.547	1.24358	2	9	4
171	76.627	1.24249	1	11	4
172	76.655	1.24211	4	2	1
173	76.757	1.24071	3	4	4

174	76.81	1.23998	3	9	2
175	77.006	1.23731	2	11	3
176	77.221	1.2344	1	4	6
177	77.276	1.23366	2	6	5
178	77.387	1.23217	3	10	1
179	77.679	1.22827	4	3	1
180	77.996	1.22406	2	13	1
181	78.007	1.22393	4	4	0
182	78.377	1.21907	1	9	5
183	78.63	1.21578	0	12	4
184	78.61	1.21604	0	6	6
185	78.597	1.21621	3	5	4
186	78.725	1.21455	1	14	2
187	78.72	1.21462	1	13	3
188	78.848	1.21296	3	8	3
189	79.058	1.21026	1	5	6
190	79.106	1.20965	4	4	1
191	79.144	1.20917	4	0	2
192	79.347	1.20658	4	1	2
193	79.557	1.20393	0	10	5
194	79.925	1.1993	2	7	5
195	79.956	1.19892	4	2	2

Table S3. Fractional atomic coordinates (x, y, z) and main bond lengths (Å) for the orthorhombic structure of $KY(MoO_4)_2$.

	Coordinates			Bond length			
	x	*y*	*z*				
K	0.5	0.268(1)	0.25	K-O4(×2)	2.649(5)	Mo-O1	1.787(4)
Y	0	0.0057(9)	0.25	K-O4(×2)	2.837(5)	Mo-O2	1.971(6)
Mo	0.526(7)	0.0988(4)	-0.014 (1)	K-O2(×2)	3.157 (5)	Mo-O3	1.815(5)
O1	0.790(7)	0.094(2)	0.134(6)	Y-O1(×2)	2.163(5)	Mo-O4	1.841(5)
O2	0.801(1)	0.072(2)	-0.179(9)	Y-O2(×2)	1.849(5)		
O3	0.232(1)	0.044(2)	0.016(1)	Y-O3(×2)	2.310(7)		
O4	0.389(1)	0.189(2)	-0.049(6)	Y-O3(×2)	2.590(7)		

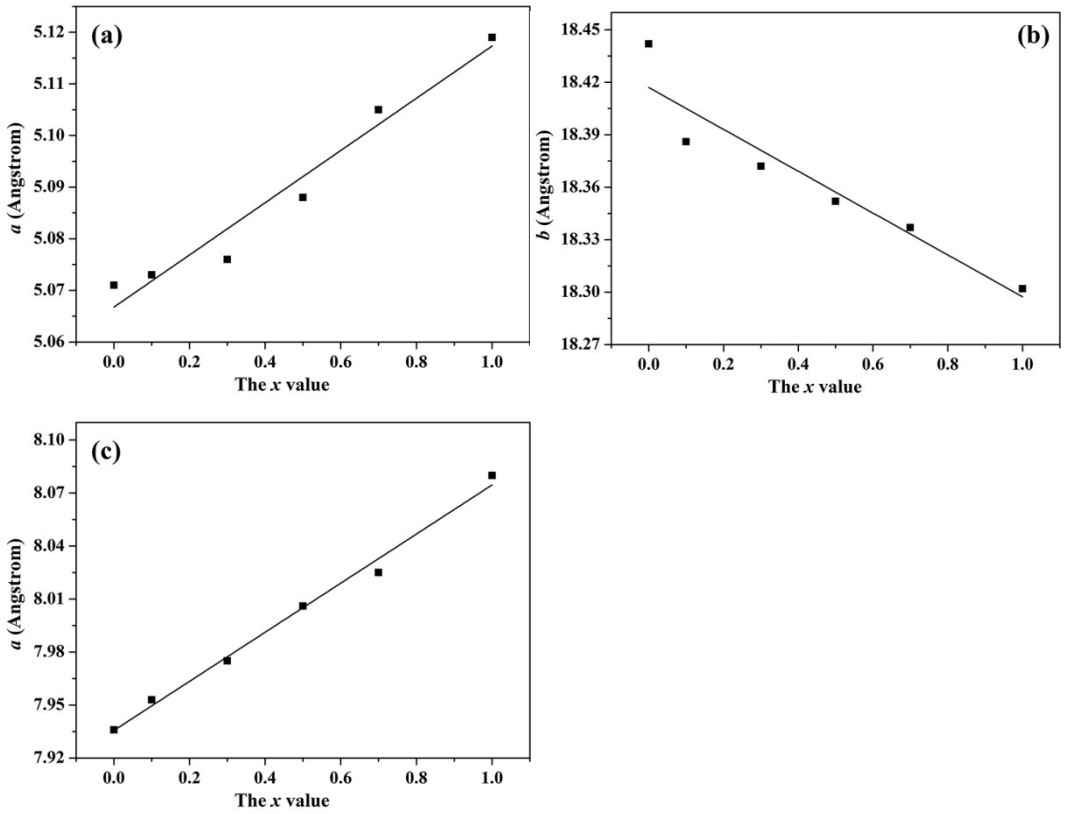

Fig. S4. The correlation of lattice parameters *a* (a), *b* (b) and c (*c*) with the Eu content (*x* value) for orthorhombic $KY_{1-x}Eu_x(MoO_4)_2$.

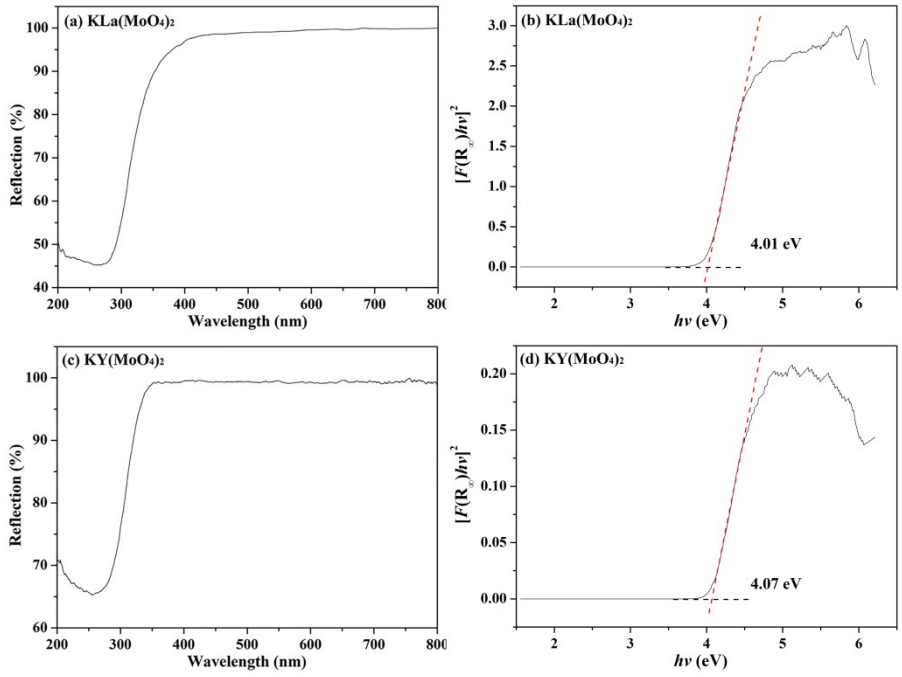

Fig. S5. Diffuse reflectance spectra (a, c) and $[F(R_\infty)h\nu]^2$ versus $h\nu$ plots (b, d) for monoclinic $KLa(MoO_4)_2$ (a, b) and orthorhombic $KY(MoO_4)_2$ (c, d).

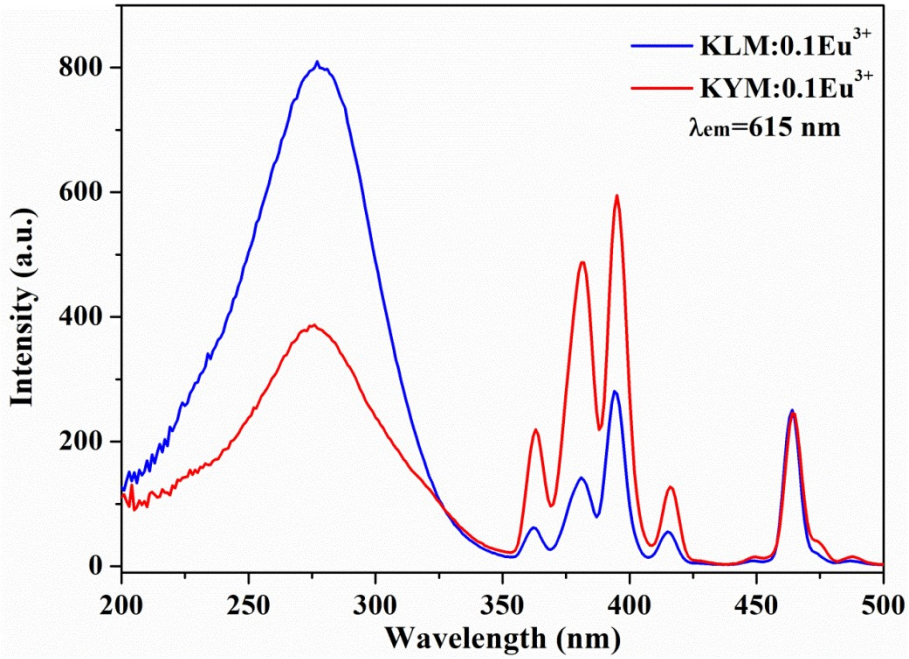

Fig. S6. PLE spectra of the KLM:0.1Eu and KYM:0.1Eu phosphors.

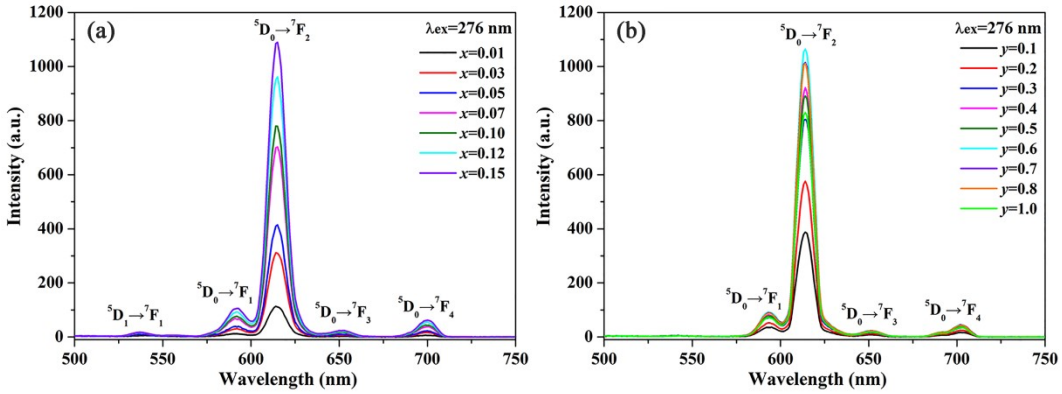

Fig. S7. PL spectra of the KLM:*x*Eu (a) and KYM:*y*Eu (b) phosphors under 276 nm excitation.

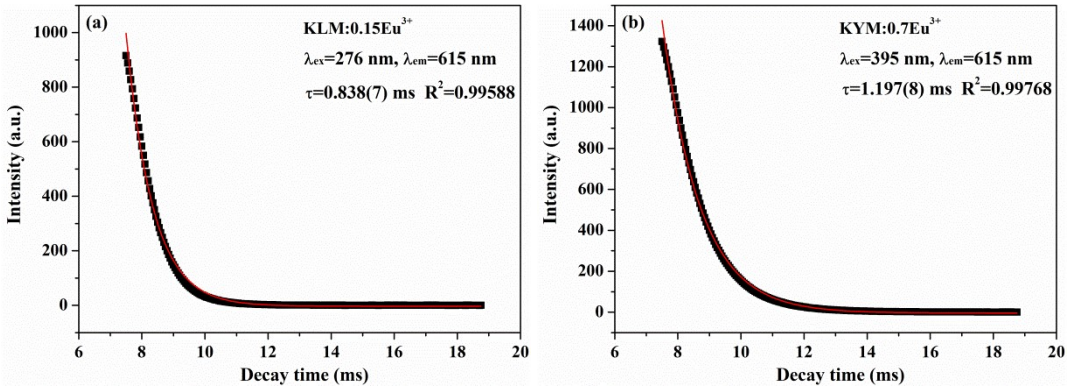

Fig. S8. Fluorescence decay curves for the 615 nm emission of KLM:0.15Eu (a) and KYM:0.7Eu (b).

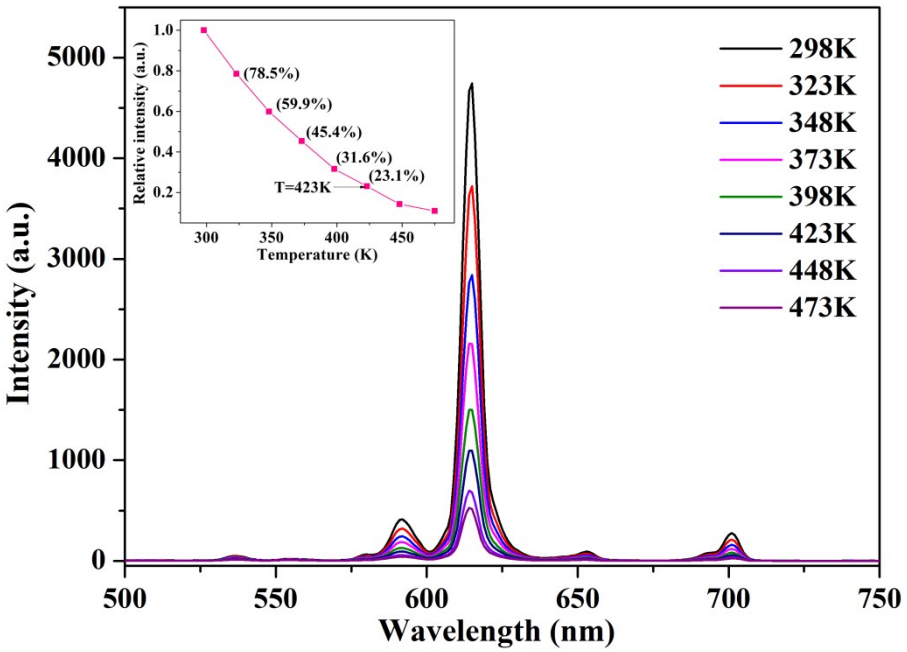

Fig. S9. Temperature-dependent PL spectra of the KLM:0.15Eu^{3+} phosphor (λ_{ex}=276 nm; 298-473 K). The inset shows the relative intensity of the 615 nm emission