

## Supplementary data

### Triple molybdate scheelite-type upconversion phosphor

### **NaCaLa(MoO<sub>4</sub>)<sub>3</sub>:Er<sup>3+</sup>/Yb<sup>3+</sup>: structural and spectroscopic properties**

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**Table 1S.** Fractional atomic coordinates and isotropic displacement parameters ( $\text{\AA}^2$ ) of NCLM: $x\text{Er}^{3+}$ , $y\text{Yb}^{3+}$  samples

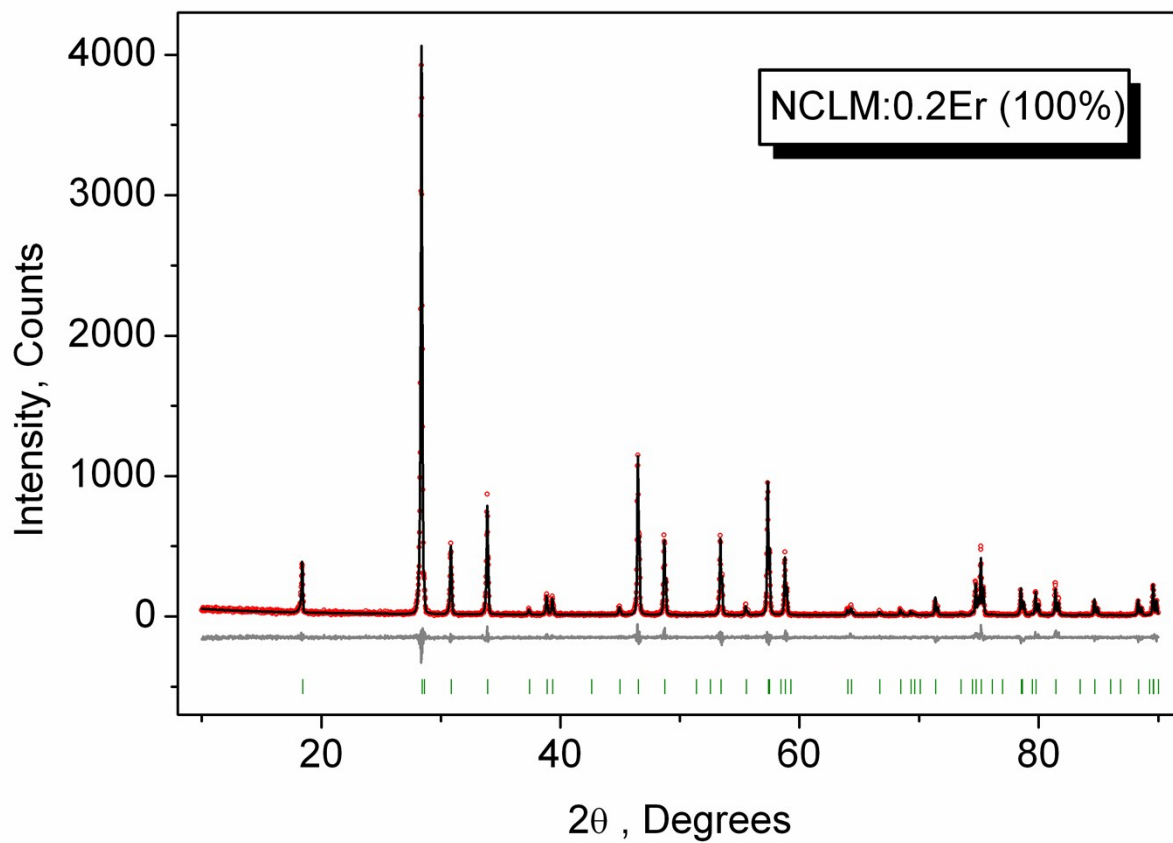
	$x$	$y$	$z$	$B_{\text{iso}}$	Occ.
NCLM					
Na	0	1/4	5/8	0.8 (2)	1/3
Ca	0	1/4	5/8	0.8 (2)	1/3
La	0	1/4	5/8	0.8 (2)	1/3
Mo	0	1/4	1/8	0.5 (2)	1
O	0.253 (2)	0.119 (2)	0.0450 (8)	0.5 (3)	1
NCLM:0.2Er <sup>3+</sup>					
Na	0	1/4	5/8	0.7 (2)	1/3
Ca	0	1/4	5/8	0.7 (2)	1/3
La	0	1/4	5/8	0.7 (2)	4/15
Er	0	1/4	5/8	0.7 (2)	1/15
Mo	0	1/4	1/8	0.5 (2)	1
O	0.240 (2)	0.108 (1)	0.0436 (7)	0.5 (3)	1
NCLM:0.1Er <sup>3+</sup> ,0.2Yb <sup>3+</sup>					
Na	0	1/4	5/8	0.6 (2)	1/3
Ca	0	1/4	5/8	0.6 (2)	1/3
La	0	1/4	5/8	0.6 (2)	7/30
Er	0	1/4	5/8	0.6 (2)	1/30
Yb	0	1/4	5/8	0.6 (2)	2/30
Mo	0	1/4	1/8	0.5 (2)	1
O	0.241 (2)	0.103 (1)	0.0399 (6)	0.8 (3)	1
NCLM:0.05Er <sup>3+</sup> ,0.45Yb <sup>3+</sup>					
Na	0	1/4	5/8	0.5 (2)	1/3

Ca	0	1/4	5/8	0.5 (2)	1/3
La	0	1/4	5/8	0.5 (2)	10/60
Er	0	1/4	5/8	0.5 (2)	1/60
Yb	0	1/4	5/8	0.5 (2)	9/60
Mo	0	1/4	1/8	0.5 (2)	1
O	0.241 (2)	0.102 (1)	0.0420 (6)	0.5 (3)	1

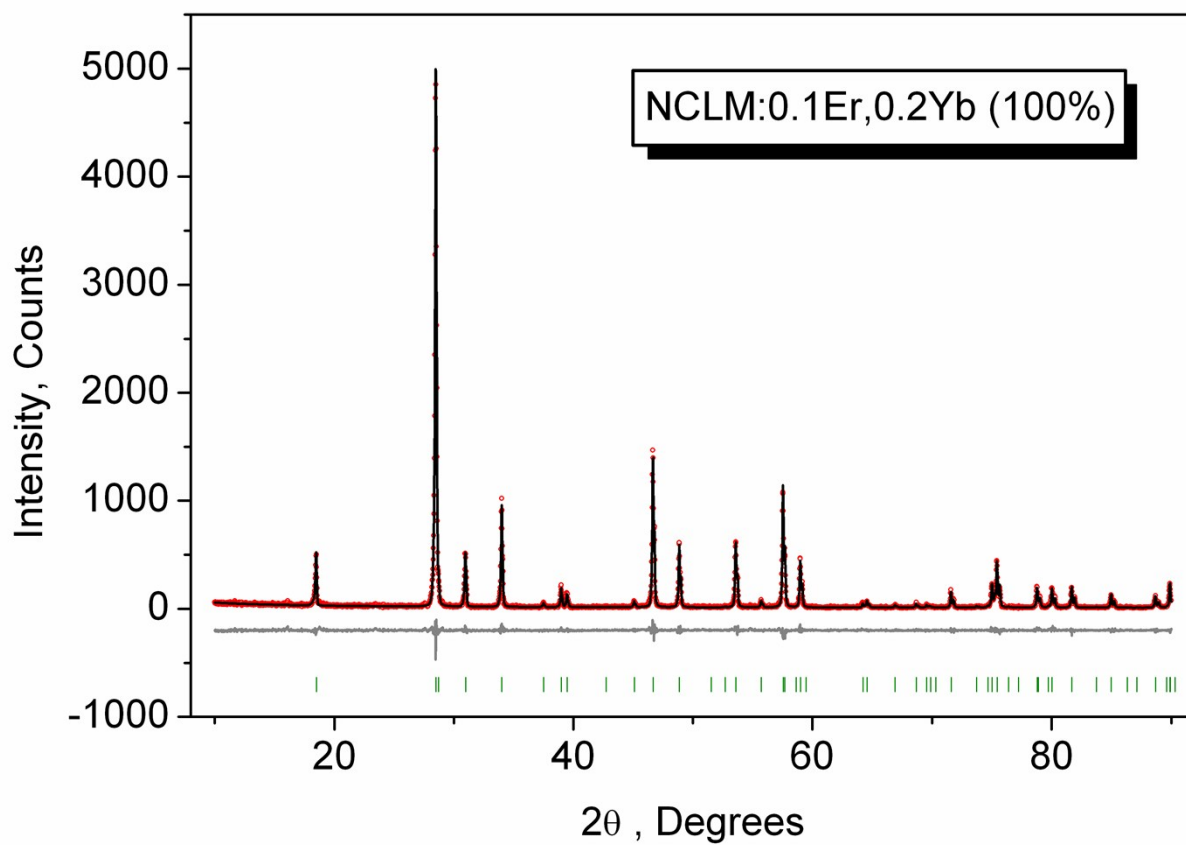
**Table 2S.** Main bond lengths (Å) of NCLM: $x\text{Er}^{3+}$ , $y\text{Yb}^{3+}$  samples

NCLM			
(Na/Ca/La)—O <sup>i</sup>	2.53 (1)	Mo—O	1.77 (1)
(Na/Ca/La)—O <sup>ii</sup>	2.47 (1)		
NCLM:0.2Er <sup>3+</sup>			
(Na/Ca/La/Er)—O <sup>i</sup>	2.518 (9)	Mo—O	1.749 (9)
(Na/Ca/La/Er)—O <sup>ii</sup>	2.502 (9)		
NCLM:0.1Er <sup>3+</sup> ,0.2Yb <sup>3+</sup>			
(Na/Ca/La/Er/Yb)—O <sup>i</sup>	2.505 (9)	Mo—O	1.782 (9)
(Na/Ca/La/Er/Yb)—O <sup>ii</sup>	2.467 (9)		
NCLM:0.05Er <sup>3+</sup> ,0.45Yb <sup>3+</sup>			
(Na/Ca/La/Er/Yb)—O <sup>i</sup>	2.482 (9)	Mo—O	1.760 (9)
(Na/Ca/La/Er/Yb)—O <sup>ii</sup>	2.474 (8)		

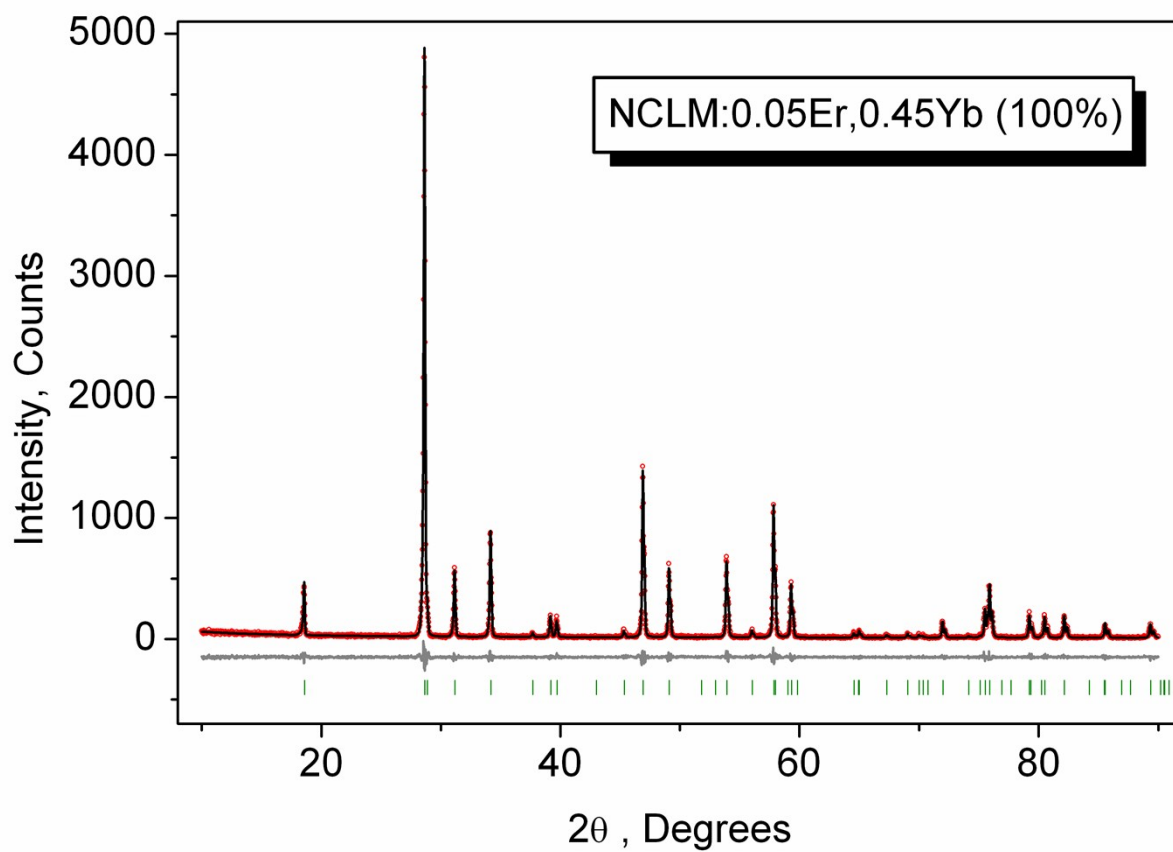
Symmetry codes: (i)  $-x+1/2, -y, z+1/2$ ; (ii)  $-x+1/2, -y+1/2, -z+1/2$ .



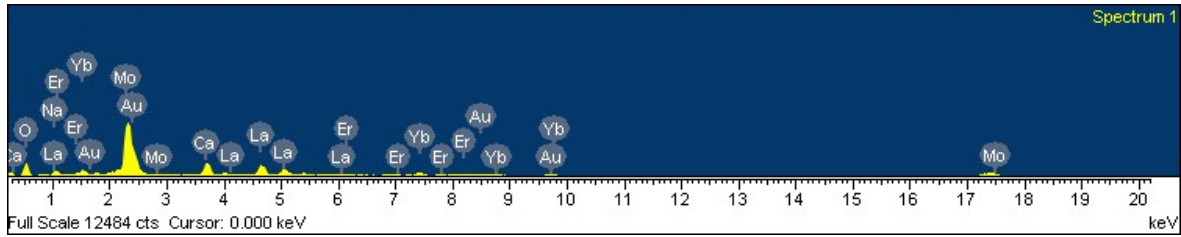
**Figure 1S.** Difference Rietveld plot of NCLM:0.2Er<sup>3+</sup>.



**Figure 2S.** Difference Rietveld plot of NCLM:0.1Er<sup>3+</sup>,0.2Yb<sup>3+</sup>.



**Figure 3S.** Difference Rietveld plot of NCLM:0.05Er<sup>3+</sup>,0.45Yb<sup>3+</sup>.



**Figure 4S.** Energy-dispersive X-ray spectroscopy patterns of the synthesized NCLM:0.1Er<sup>3+</sup>,0.2Yb<sup>3+</sup> particles.

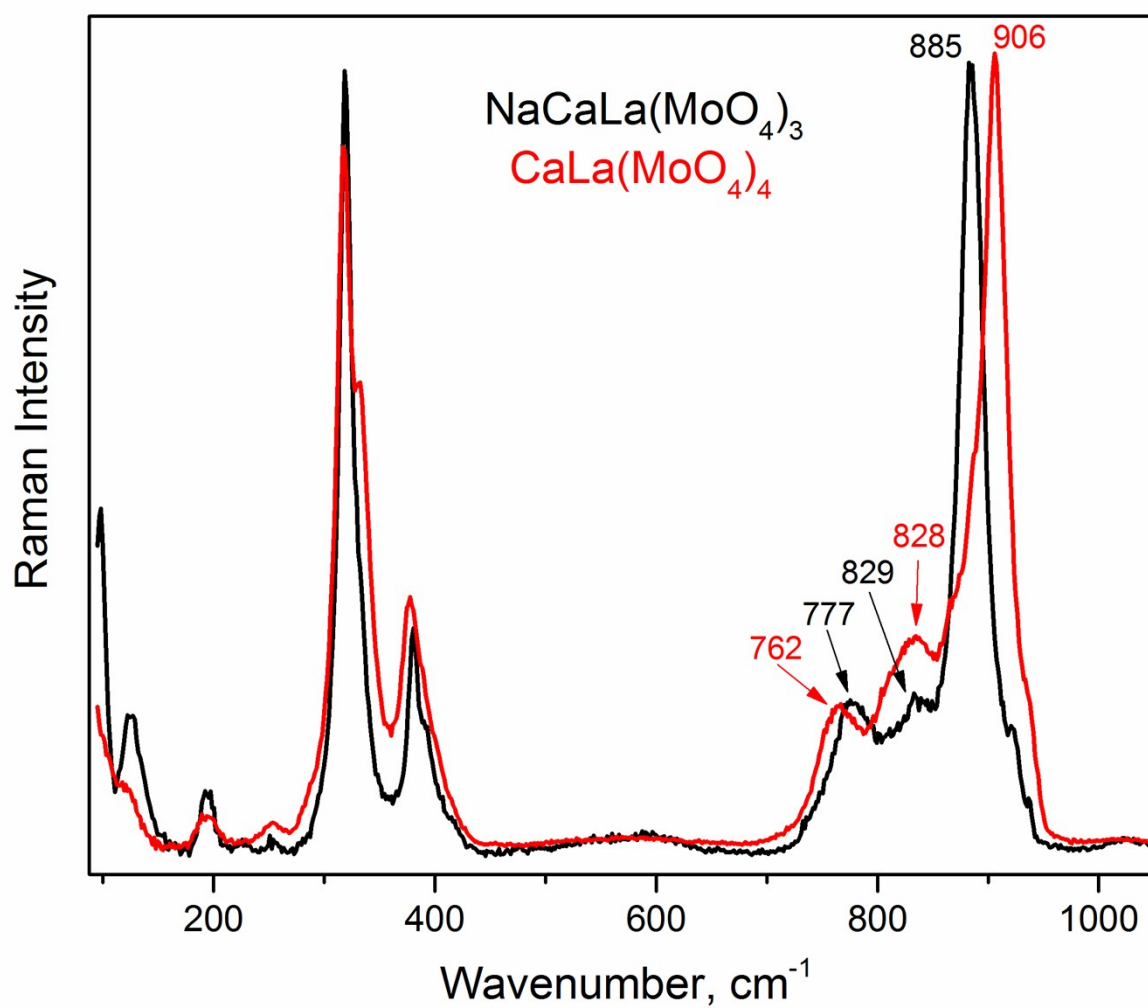
**Table 3S.** Quantitative compositions of NCLM:0.1Er<sup>3+</sup>,0.2Yb<sup>3+</sup> sample

Spectrum	In stats.	O	Na	Ca	Mo	La	Er	Yb	Total
Spectrum 1	Yes	31.99	2.59	4.65	37.48	13.35	2.51	7.43	100.00
Spectrum 2	Yes	31.53	2.88	4.56	38.47	13.82	2.10	6.63	100.00
Spectrum 3	Yes	33.03	2.81	4.49	36.10	13.94	2.31	7.32	100.00
Spectrum 4	Yes	32.39	2.61	4.30	37.45	13.66	2.57	7.02	100.00
Mean		32.24	2.72	4.50	37.37	13.69	2.37	7.10	100.00
Std. deviation		0.64	0.14	0.15	0.97	0.25	0.21	0.36	
Max.		33.03	2.88	4.65	38.47	13.94	2.57	7.43	
Min.		31.53	2.59	4.30	36.10	13.35	2.10	6.63	
Nominal values		27.75	3.33	5.80	41.64	14.07	2.41	5.00	100.00

**Table 4S.** Parameters of the interatomic interaction potential

Interaction	Radii of interaction, Å	$\lambda$ , aJ/Å <sup>2</sup>	$\rho$ , Å
Na – O	0.0 – 3.0	574.03	0.3183
Ca – O	0.0 – 3.0	714.87	0.2691
La – O	0.0 – 3.0	786.35	0.2240
Mo – O	0.0 – 2.0	176.17	0.4577
O – O (intra)	2.800 – 2.835	331.81	0.4494
O – O (intra)	3.000 – 3.025	526.57	0.4842
O – O (inter)	2.837 – 2.999	615.31	0.3670
O – O (inter)	3.025 – 3.100	612.27	0.3804
O – O (inter)	3.110 – 3.160	549.39	0.3434





**Figure 5S.** Comparison of Raman spectra of pure NCLM and CaLa<sub>2</sub>(MoO<sub>4</sub>)<sub>4</sub> [42].