Supplementary materials

Structural and spectroscopic effects of Li^+ substitution for Na^+ in $Li_xNa_{1-x}CaLa_{0.5}Er_{0.05}Yb_{0.45}(MoO_4)_3$ scheelite-type upconversion phosphors

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Table S1. Fractional atomic coordinates and isotropic displacement parameters (Å^2) of the ($Na_{1-x}Li_x$)$Ca(La_{0.5}Er_{0.05}Yb_{0.45})(MoO_4)_3$ samples

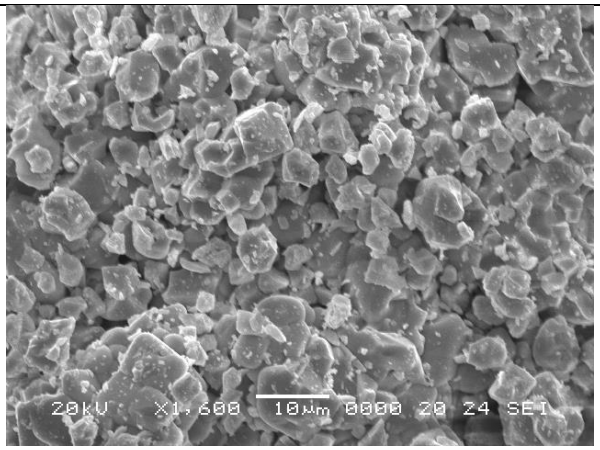
	x	*y*	*z*	B_{iso}	Occ.
NCLM					
Na	0	1/4	5/8	0.3 (2)	1/3
Ca	0	1/4	5/8	0.3 (2)	1/3
La	0	1/4	5/8	0.3 (2)	1/6
Er	0	1/4	5/8	0.3 (2)	1/60
Yb	0	1/4	5/8	0.3 (2)	0.15
Mo	0	1/4	5/8	0.5 (2)	1
O	0.240 (2)	0.103 (2)	0.0429 (7)	0.7 (3)	1
$Na_{0.95}Li_{0.05}$CLM:0.05Er,0.45Yb					
Na	0	1/4	5/8	0.7 (2)	19/60
Li	0	1/4	5/8	0.7 (2)	1/60
Ca	0	1/4	5/8	0.7 (2)	1/3
La	0	1/4	5/8	0.7 (2)	1/6
Er	0	1/4	5/8	0.7 (2)	1/60
Yb	0	1/4	5/8	0.7 (2)	0.15
Mo	0	1/4	1/8	0.5 (2)	1
O	0.239 (2)	0.102 (1)	0.0432 (6)	0.5 (3)	1
$Na_{0.9}Li_{0.1}$CLM:0.05Er,0.45Yb					
Na	0	1/4	5/8	1.4 (2)	3/10
Li	0	1/4	5/8	1.4 (2)	1/30
Ca	0	1/4	5/8	1.4 (2)	1/3
La	0	1/4	5/8	1.4 (2)	1/6
Er	0	1/4	5/8	1.4 (2)	1/60
Yb	0	1/4	5/8	1.4 (2)	0.15
Mo	0	1/4	1/8	1.3 (2)	1
O	0.235 (2)	0.107 (1)	0.0453 (7)	1.2 (3)	1
$Na_{0.8}Li_{0.2}$CLM:0.05Er,0.45Yb					
Na	0	1/4	5/8	0.5 (2)	8/30
Li	0	1/4	5/8	0.5 (2)	2/30
Ca	0	1/4	5/8	0.5 (2)	1/3
La	0	1/4	5/8	0.5 (2)	1/6

Er	0	1/4	5/8	0.5 (2)	1/60
Yb	0	1/4	5/8	0.5 (2)	0.15
Mo	0	1/4	1/8	0.6 (2)	1
O	0.245 (2)	0.096 (1)	0.0395 (6)	0.5 (3)	1
$Na_{0.7}Li_{0.3}$CLM:0.05Er,0.45Yb					
Na	0	1/4	5/8	1.0 (2)	7/30
Li	0	1/4	5/8	1.0 (2)	1/10
Ca	0	1/4	5/8	1.0 (2)	1/3
La	0	1/4	5/8	1.0 (2)	1/6
Er	0	1/4	5/8	1.0 (2)	1/60
Yb	0	1/4	5/8	1.0 (2)	0.15
Mo	0	1/4	1/8	0.8 (2)	1
O	0.234 (2)	0.103 (1)	0.0415 (6)	1.1 (3)	1

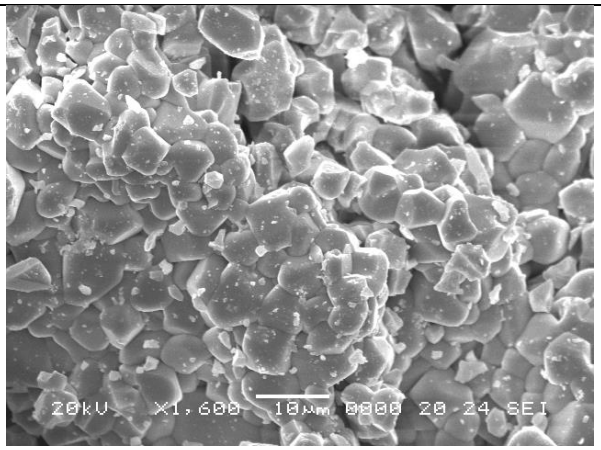
Table S2. Main bond lengths (Å) of the $(Na_{1-x}Li_x)Ca(La_{0.5}Er_{0.05}Yb_{0.45})(MoO_4)_3$ samples

NCLM			
(Na/Ca/La)—O^{i}	2.48 (1)	Mo—O	1.75 (1)
(Na/Ca/La)—O^{ii}	2.48 (1)		
$Na_{0.95}Li_{0.05}$CLM:0.05Er,0.45Yb			
(Na//Li/Ca/La/Er/Yb)—O^{i}	2.483 (9)	Mo—O	1.746 (8)
(Na//Li/Ca/La/Er/Yb)—O^{ii}	2.490 (8)		
$Na_{0.9}Li_{0.1}$CLM:0.05Er,0.45Yb			
(Na//Li/Ca/La/Er/Yb)—O^{i}	2.50 (1)	Mo—O	1.71 (1)
(Na//Li/Ca/La/Er/Yb)—O^{ii}	2.511 (9)		
$Na_{0.8}Li_{0.2}$CLM:0.05Er,0.45Yb			
(Na//Li/Ca/La/Er/Yb)—O^{i}	2.45 (1)	Mo—O	1.824 (9)
(Na//Li/Ca/La/Er/Yb)—O^{ii}	2.431 (9)		
$Na_{0.7}Li_{0.3}$CLM:0.05Er,0.45Yb			
(Na//Li/Ca/La/Er/Yb)—O^{i}	2.505 (9)	Mo—O	1.735 (9)
(Na//Li/Ca/La/Er/Yb)—O^{ii}	2.482 (8)		

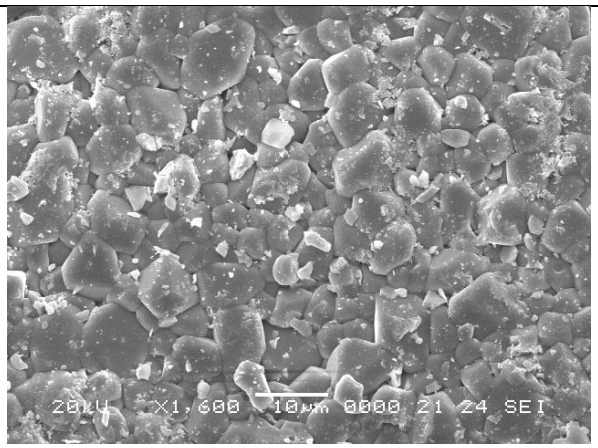
Symmetry codes: (i) $-x+1/2, -y, z+1/2$; (ii) $-x+1/2, -y+1/2, -z+1/2$.



a

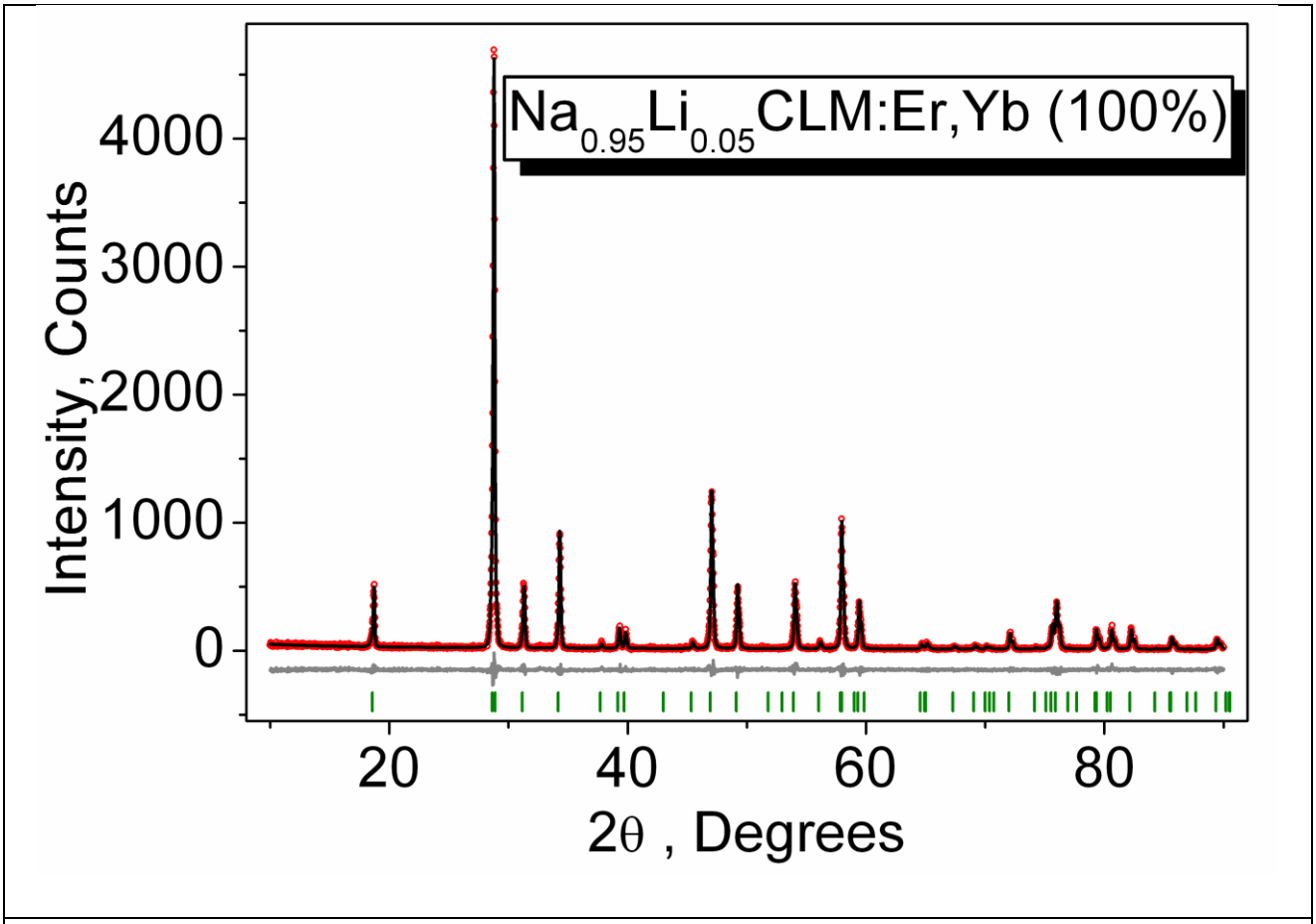


b

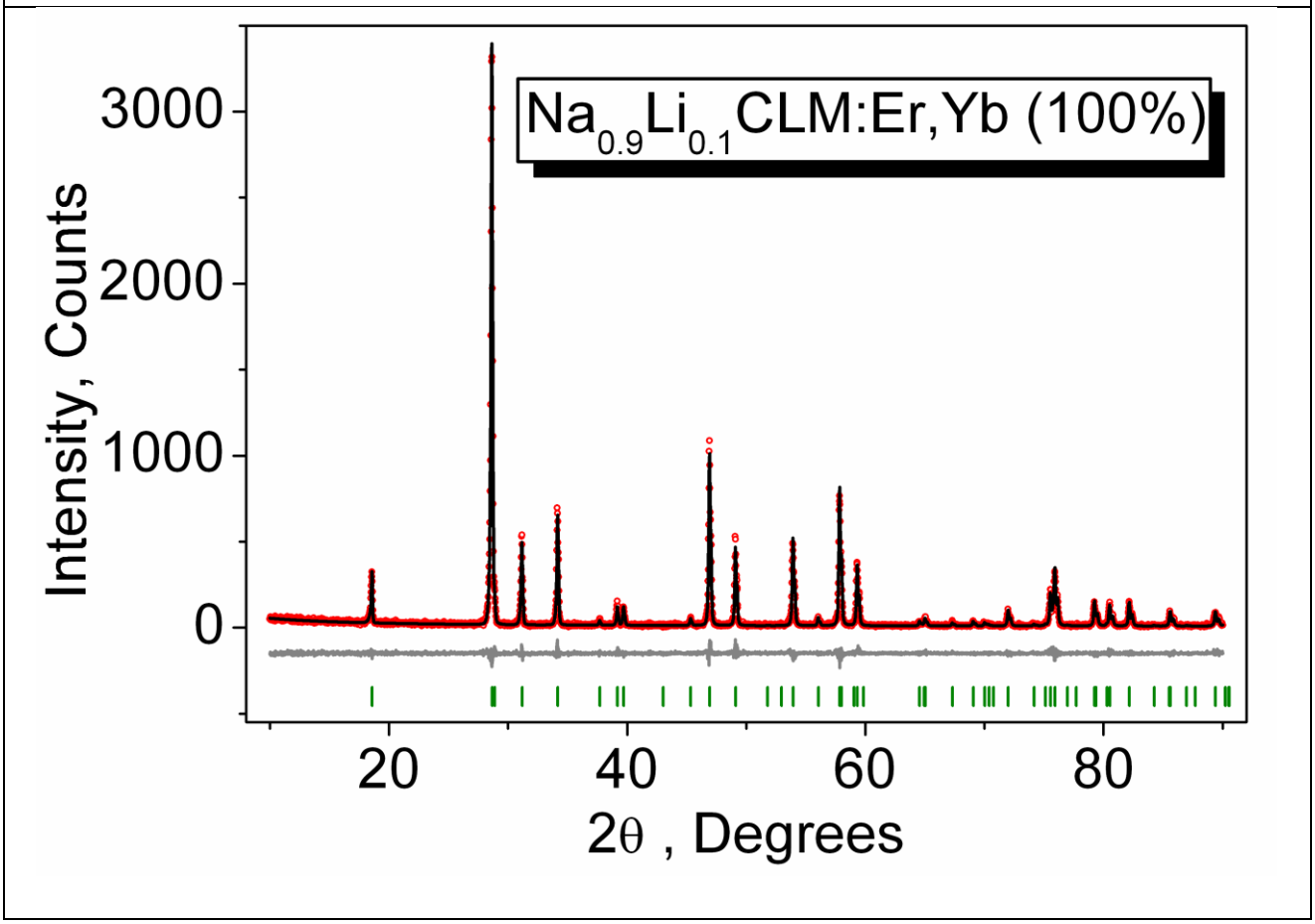


c

Figure S1. SEM patterns recorded for (a) LiNCLM:EY-0.05, (b) LiNCLM:EY-0.1 and (c) LiNCLM:EY-0.2.


Na0.95Li0.05CLM:Er,Yb (100%)
Intensity, Counts
4000
3000
2000
1000
0
20
40
60
80
2θ , Degrees

a


Na0.9Li0.1CLM:Er,Yb (100%)
Intensity, Counts
3000
2000
1000
0
20
40
60
80
2θ , Degrees

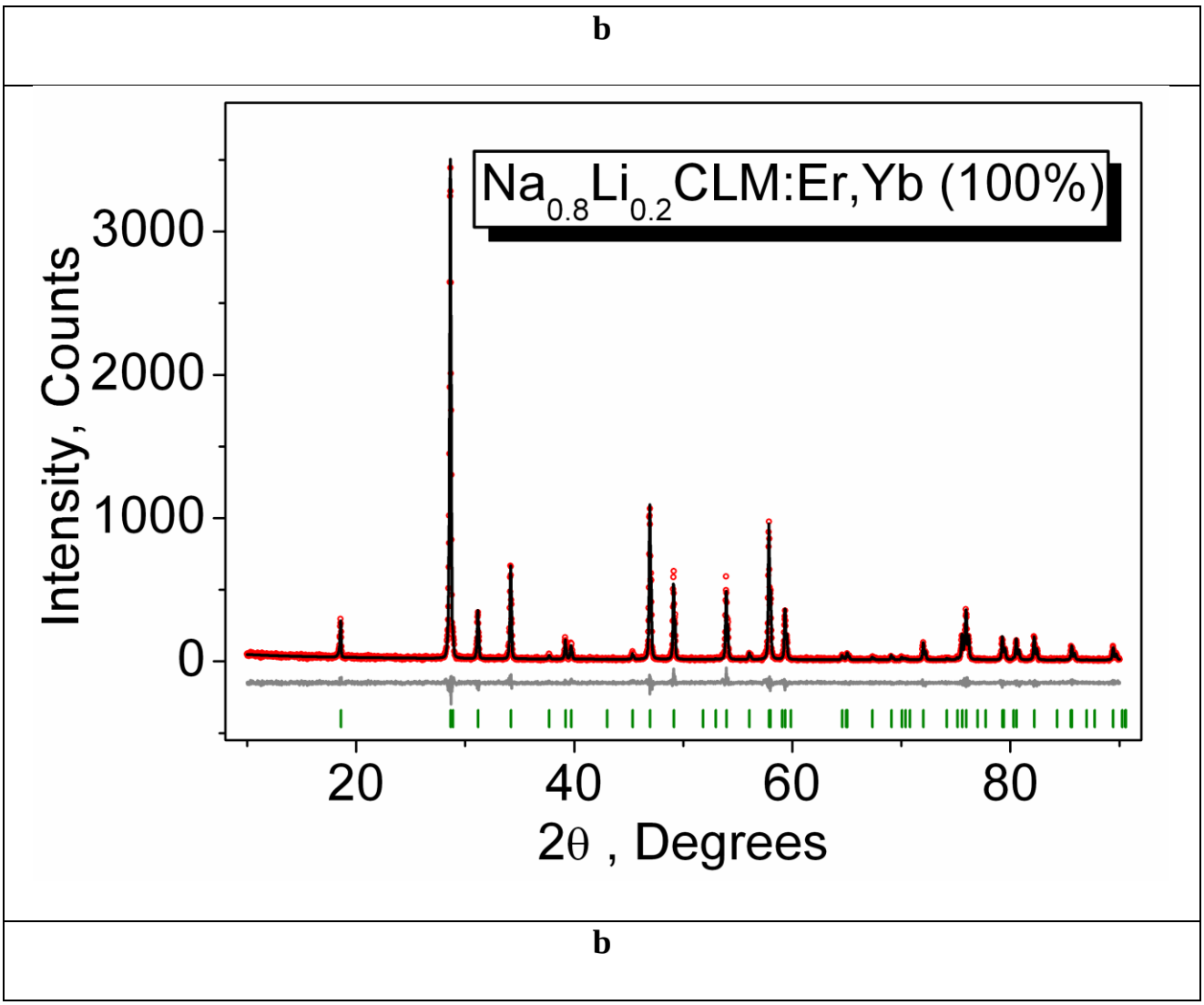


Figure S2. Rietveld difference patterns obtained for (a) LiNCLM:EY-0.05, (b) LiNCLM:EY-0.1 and (c) LiNCLM:EY-0.2. Measured points are given in red, calculated profile – in black, difference profile – in grey, and calculated peak positions are shown by segments in green.