Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementory Information

The modulated structure and frequency upconversion properties of $CaLa_2(MoO_4)_4:Ho^{3+}/Yb^{3+}$ phosphors prepared by microwave synthesis

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Table 1S. Fractional atomic coordinates and isotropic displacement parameters (Å^2) of $CaLa_{2-x}(MoO_4)_4$:Yb_y/Ho_z samples with average structure

	x	*y*	*z*	B_{iso}	Occ.
			$CaLa_2(MoO_4)_4$		
Ca	0	0.25	0.625	0.3 (3)	0.25
La	0	0.25	0.625	0.3 (3)	0.5
Mo	0	0.25	0.125	0.8 (3)	1
O	0.220 (4)	0.111 (3)	0.0443 (11)	1.2 (4)	1
			$CaLa_{1.6}(MoO_4)_4$:0.35Yb,0.05Ho		
Ca	0	0.25	0.625	1.46 (18)	0.25
La	0	0.25	0.625	1.46 (18)	0.4
Yb	0	0.25	0.625	1.46 (18)	0.0875
Ho	0	0.25	0.625	1.46 (18)	0.0125
Mo	0	0.25	0.125	1.13 (17)	1
O	0.237 (3)	0.102 (2)	0.0401 (8)	3.0 (4)	1
			$CaLa_{1.55}(MoO_4)_4$:0.4Yb,0.05Ho		
Ca	0	0.25	0.625	1.0 (2)	0.25
La	0	0.25	0.625	1.0 (2)	0.3875
Yb	0	0.25	0.625	1.0 (2)	0.1
Ho	0	0.25	0.625	1.0 (2)	0.0125
Mo	0	0.25	0.125	0.83 (18)	1
O	0.220 (3)	0.108 (2)	0.0465 (10)	1.4 (3)	1
			$CaLa_{1.5}(MoO_4)_4$:0.45Yb,0.05Ho		
Ca	0	0.25	0.625	1.14 (19)	0.25
La	0	0.25	0.625	1.14 (19)	0.375
Yb	0	0.25	0.625	1.14 (19)	0.1125
Ho	0	0.25	0.625	1.14 (19)	0.0125
Mo	0	0.25	0.125	1.25 (19)	1
O	0.225 (3)	0.110 (2)	0.0478 (10)	1.0 (3)	1
Ca	0	0.25	0.625	0.90 (19)	0.25
La	0	0.25	0.625	0.90 (19)	0.3625
Yb	0	0.25	0.625	0.90 (19)	0.125
Ho	0	0.25	0.625	0.90 (19)	0.0125
Mo	0	0.25	0.125	0.88 (18)	1
O	0.228 (3)	0.108 (2)	0.0439 (10)	1.7 (4)	1

Table 2S. Main bond lengths (Å) of $CaLa_{2-x}(MoO_4)_4$:Yb_y/Ho_z samples with average structure

$CaLa_2(MoO_4)_4$			
(Ca/La)—O^{i}	2.618 (17)	Mo—O	1.687 (16)
(Ca/La)—O^{ii}	2.605 (15)		
$CaLa_{1.6}(MoO_4)_4$:0.35Yb,0.05Ho			
(Ca/La/Yb/Ho)—O^{i}	2.536 (14)	Mo—O	1.782 (13)
(Ca/La/Yb/Ho)—O^{ii}	2.511 (12)		
$CaLa_{1.55}(MoO_4)_4$:0.4Yb,0.05Ho			
(Ca/La/Yb/Ho)—O^{i}	2.579 (14)	Mo—O	1.666 (14)
(Ca/La/Yb/Ho)—O^{ii}	2.607 (13)		
$CaLa_{1.5}(MoO_4)_4$:0.45Yb,0.05Ho			
(Ca/La/Yb/Ho)—O^{i}	2.567 (14)	Mo—O	1.668 (13)
(Ca/La/Yb/Ho)—O^{ii}	2.602 (13)		
$CaLa_{1.45}(MoO_4)_4$:0.5Yb,0.05Ho			
(Ca/La/Yb/Ho)—O^{i}	2.566 (16)	Mo—O	1.709 (15)
(Ca/La/Yb/Ho)—O^{ii}	2.562 (14)		

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

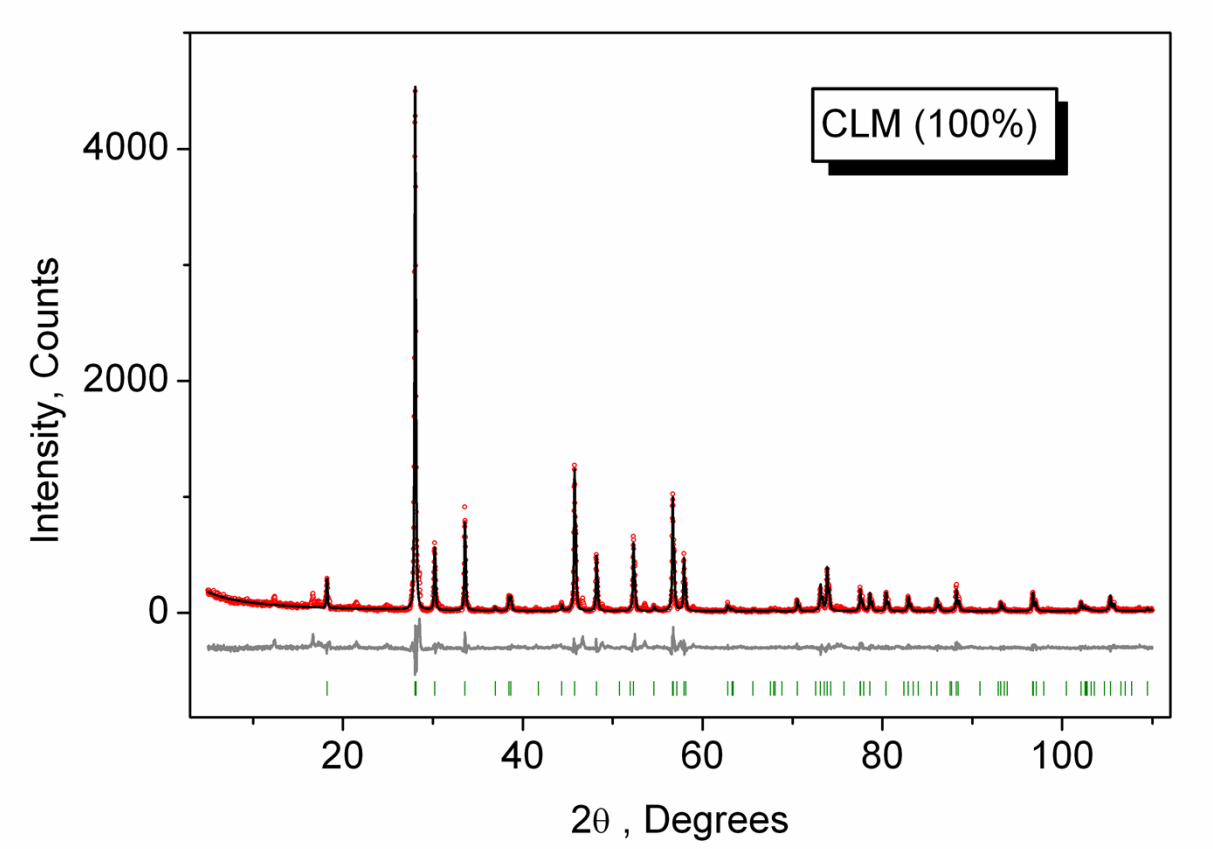

Figure 1S. Difference Rietveld plot of $CaLa_2(MoO_4)_4$ without accounting of modulated superstructure peaks.

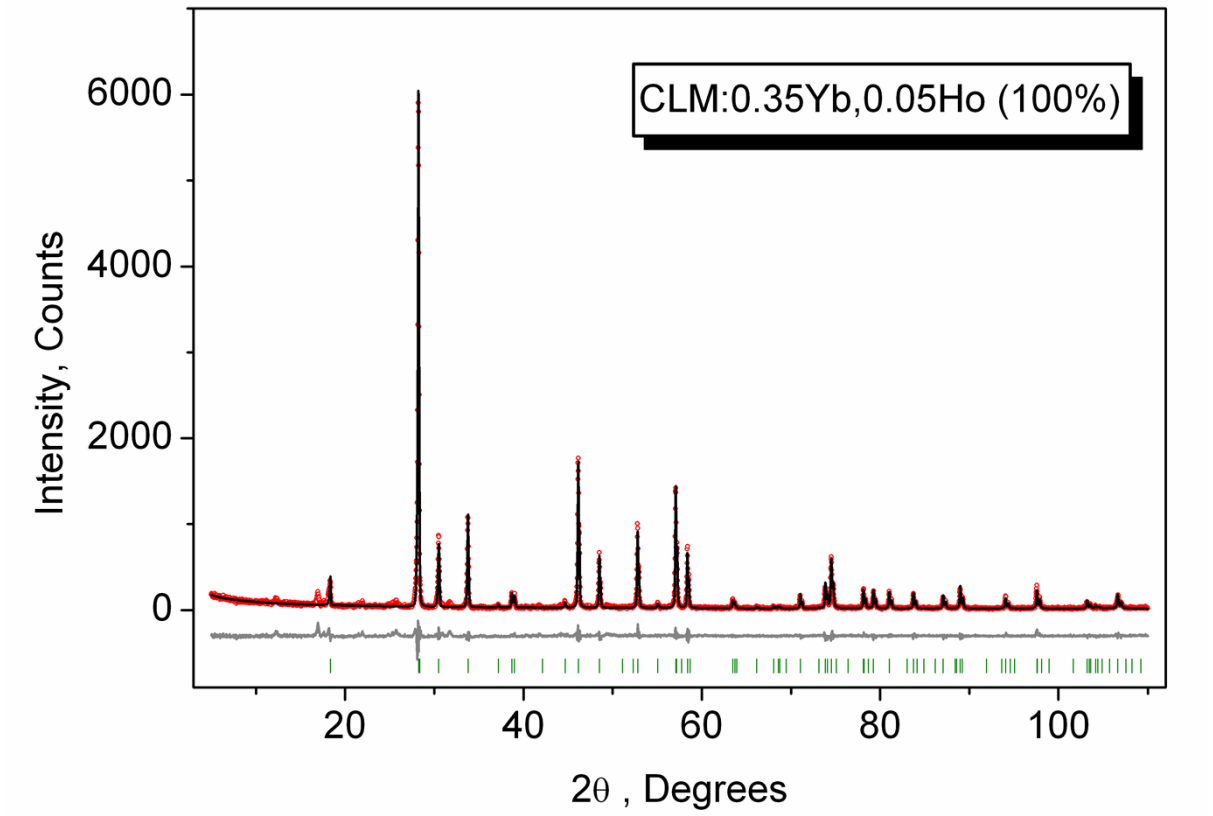

Figure 2S. Difference Rietveld plot of $CaLa_{1.6}(MoO_4)_4$:0.35Yb,0.05Ho without accounting of modulated superstructure peaks.

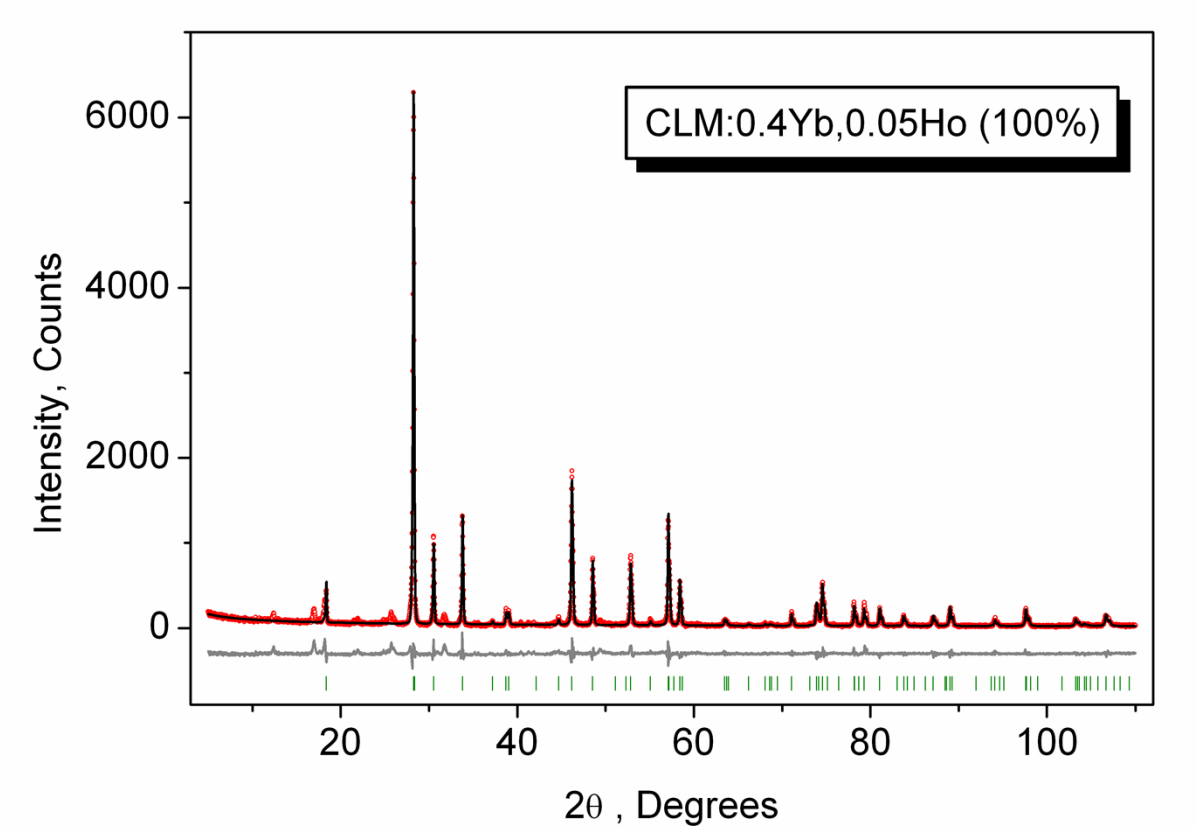

Figure 3S. Difference Rietveld plot of $CaLa_{1.55}(MoO_4)_4$:0.4Yb,0.05Ho without accounting of modulated superstructure peaks.

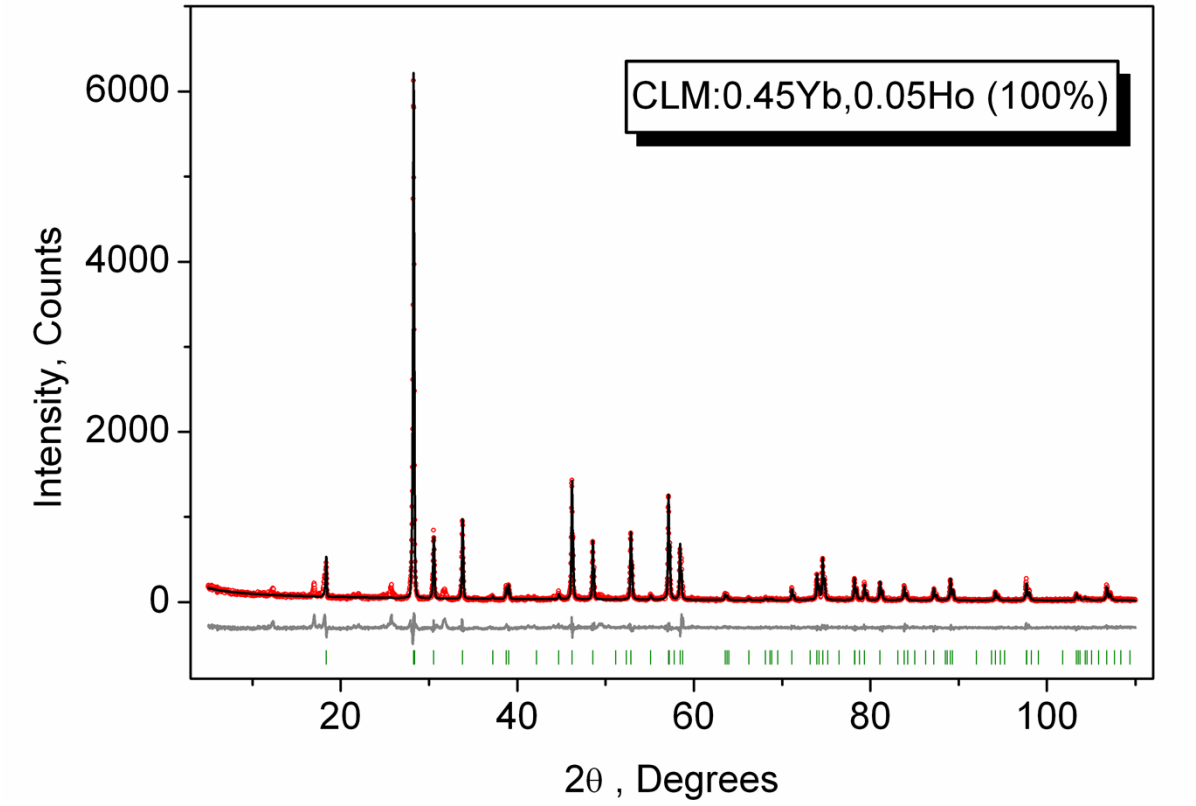

Figure 4S. Difference Rietveld plot of $CaLa_{1.5}(MoO_4)_4$:0.45Yb,0.05Ho without accounting of modulated superstructure peaks.

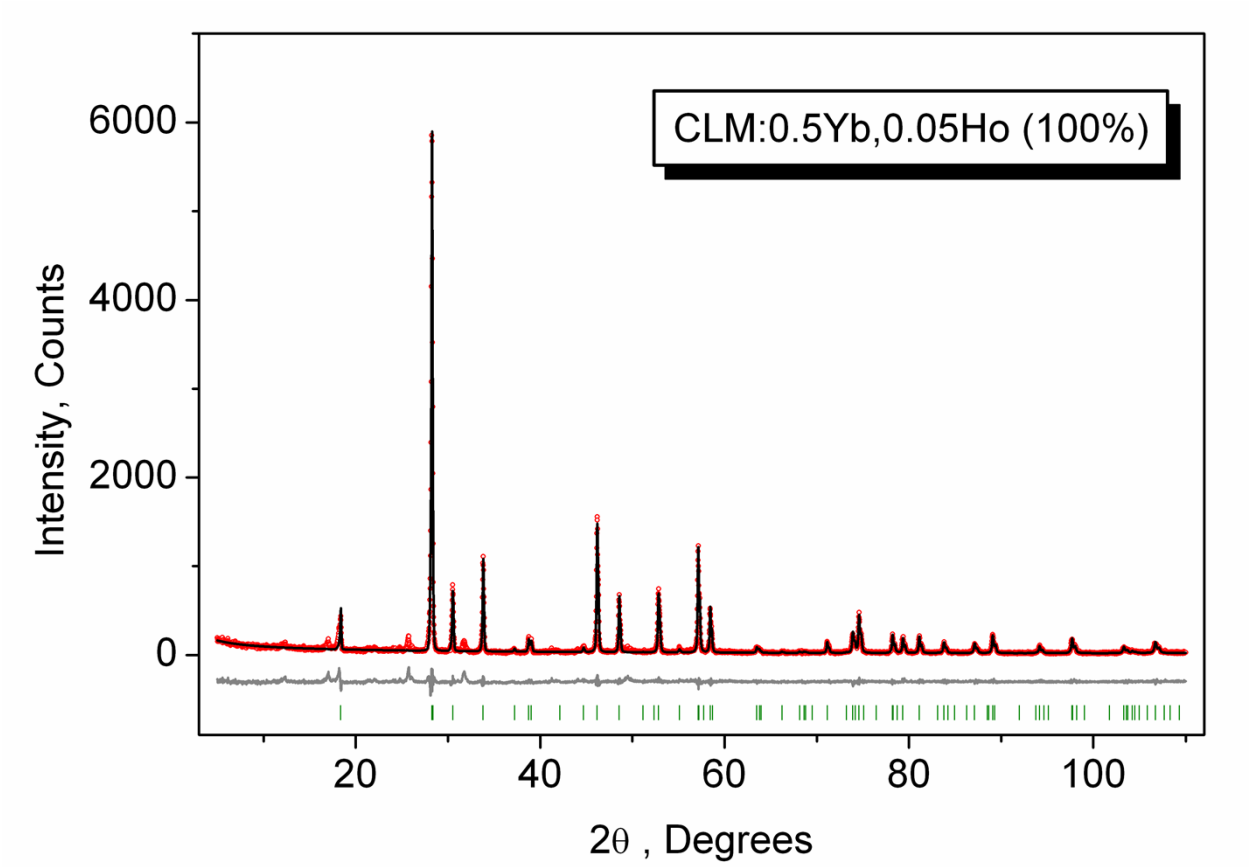

Figure 5S. Difference Rietveld plot of $CaLa_{1.45}(MoO_4)_4$:0.5Yb,0.05Ho without accounting of modulated superstructure peaks.

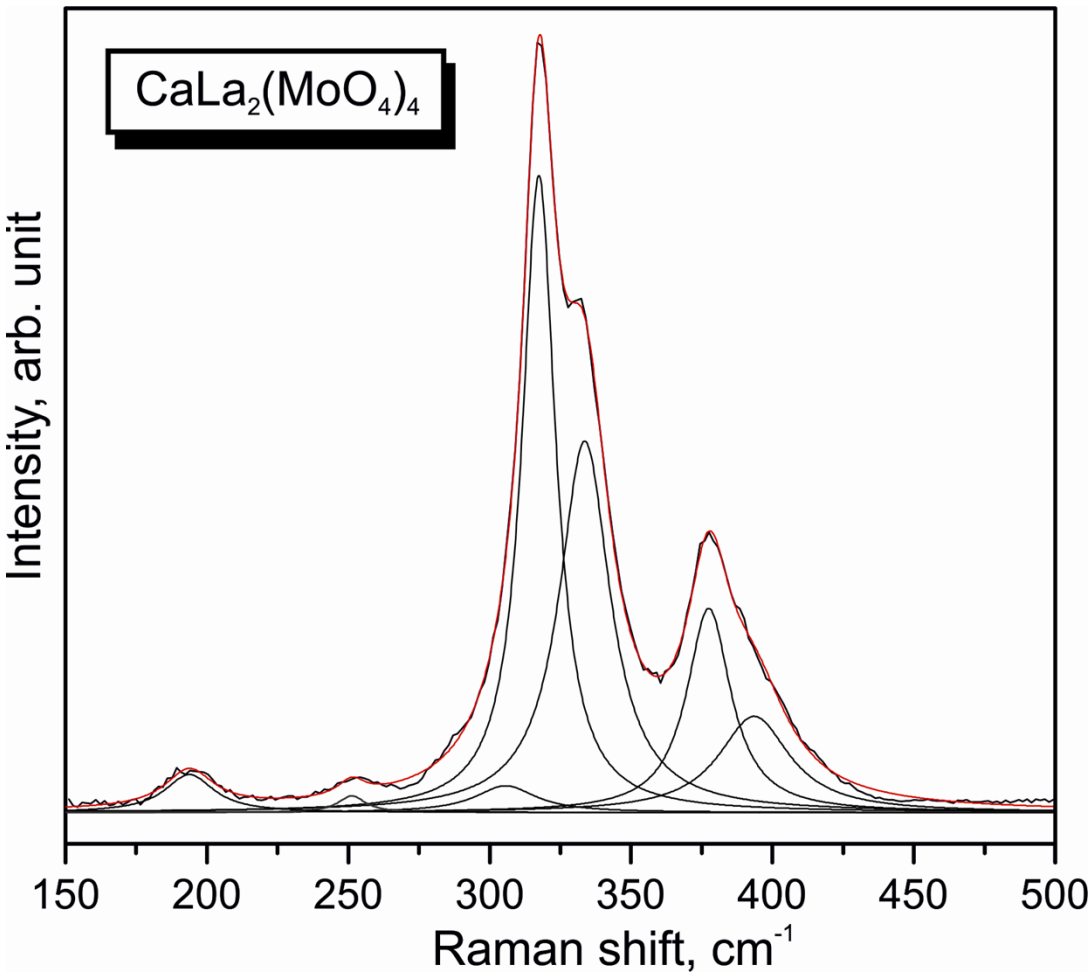

Fig. 6S. Raman spectrum of $CaLa_2(MoO_4)_4$ over the low wavenumber range.

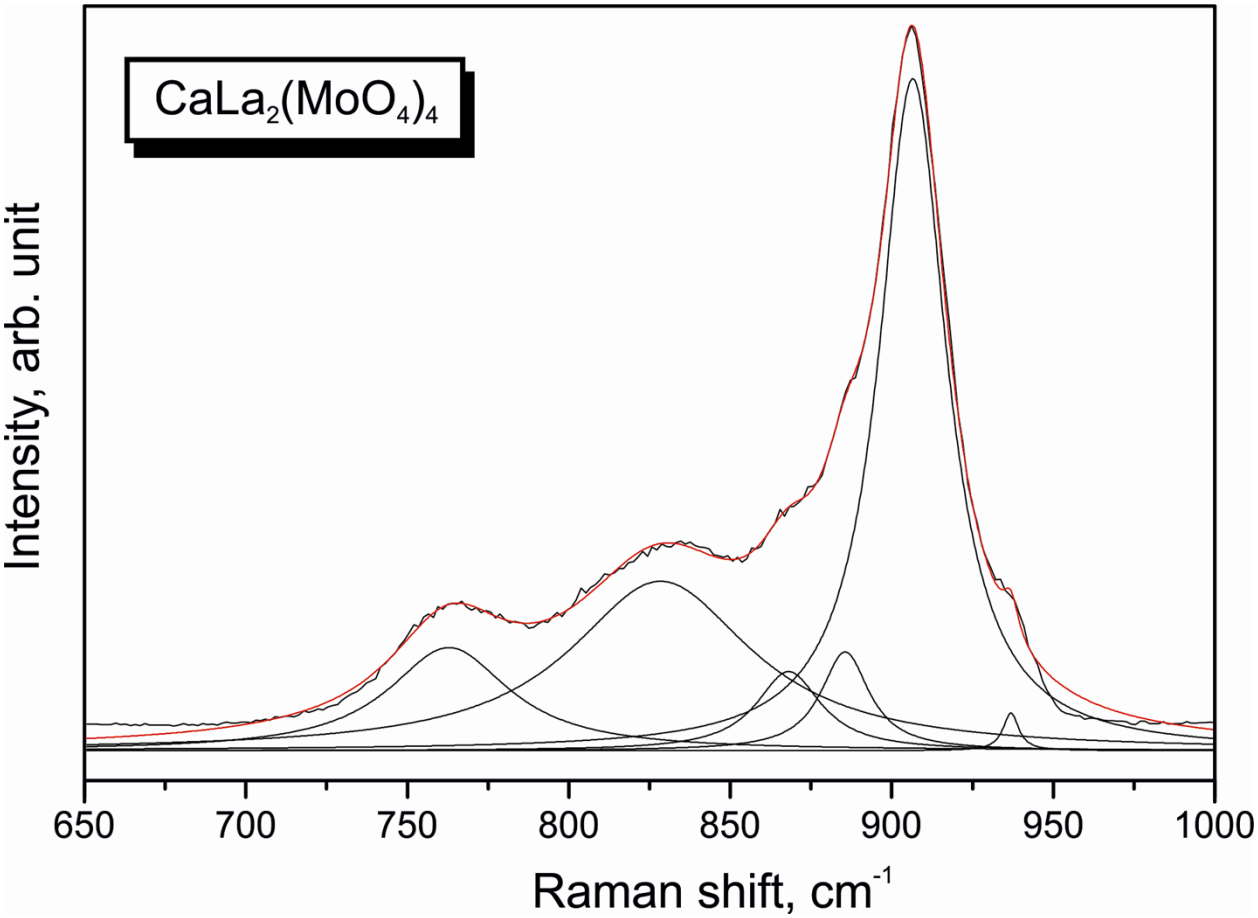

Fig. 7S. Raman spectrum of $CaLa_2(MoO_4)_4$ over the high wavenumber range.

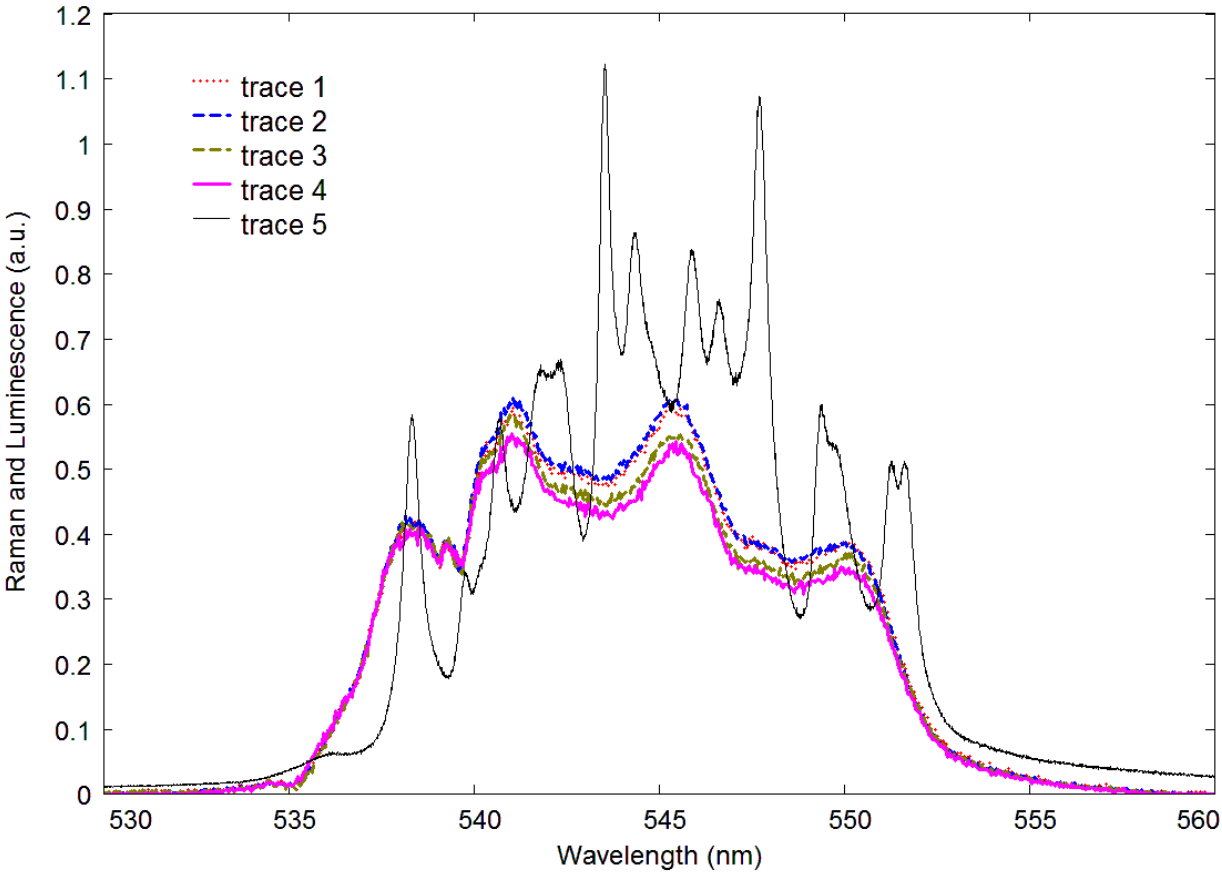

Fig. 8S. Emission spectra of $CaLa_{2-x}(MoO_4)_4$:Yb_y/Ho_z samples with the spectrum of undoped $CaLa_2(MoO_4)_4$ being extracted from all doped samples spectra. Reference spectrum of Ho ion luminescence in holmium aluminum borate ($HoAl_3(BO_3)_4$, [59]) is added for comparison.