

## Supporting Information

### Study of multimodal light emissions from Pr<sup>3+</sup>/Yb<sup>3+</sup> doped NaLa(MoO<sub>4</sub>)<sub>2</sub> phosphors for optoelectronic devices and plant-growth applications

<sup>a</sup>Sonali Tomar, <sup>b,c</sup>Neeraj Kumar Mishra, <sup>d</sup>Vaibhav Chauhan, <sup>b</sup>Kaushal Kumar, <sup>a</sup>C. Shivakumara\*

<sup>a</sup>Solid State and Structural Chemistry Unit, Indian Institute of Science,  
Bangalore - 560012, India

<sup>b</sup>Optical Materials and Bio-imaging Research Laboratory, Department of Physics,  
Indian Institute of Technology (Indian School of Mines), Dhanbad - 826004, India

<sup>c</sup>Department of Chemical Sciences, Indian Institute of Science Education and  
Research (IISER), Mohali, Punjab -140306, India

<sup>d</sup>Atomic and Molecular Physics Division, Bhabha Atomic Research Center,  
Mumbai – 400085, India

#### Contents

**Figure S1.** Rietveld plot of (a) NaLa(MoO<sub>4</sub>)<sub>2</sub>, (b) NaLa<sub>0.97</sub>Pr<sub>0.03</sub>(MoO<sub>4</sub>)<sub>2</sub> and (c) NaLa<sub>0.94</sub>Pr<sub>0.03</sub>Yb<sub>0.03</sub>(MoO<sub>4</sub>)<sub>2</sub>, (d) crystal structure of NaLa<sub>0.97</sub>Pr<sub>0.03</sub>(MoO<sub>4</sub>)<sub>2</sub> and (e) XRD patterns of NaLa<sub>0.97-y</sub>Pr<sub>0.03</sub>Yb<sub>y</sub>(MoO<sub>4</sub>)<sub>2</sub> (0.00 ≤ x ≤ 0.14) phosphors.

**Figure S2.** High-resolution XPS spectra of NaLa<sub>0.92</sub>Pr<sub>0.03</sub>Yb<sub>0.05</sub>(MoO<sub>4</sub>)<sub>2</sub>: (a) XPS scan Survey (b) Na 1s spectra (c) La 3d spectra (d) Pr 3d, (e) Yb 4d, (f) Mo 3d spectra and (g) O 1s spectra.

**Figure S3.** FTIR spectra of NaLa<sub>1-x</sub>Pr<sub>x</sub>(MoO<sub>4</sub>)<sub>2</sub> and NaLa<sub>0.97-y</sub>Pr<sub>0.03</sub>Yb<sub>y</sub>(MoO<sub>4</sub>)<sub>2</sub> phosphors.

**Figure S4.** (a) Diffusion reflectance spectra of pure, Pr<sup>3+</sup> doped and Pr<sup>3+</sup>/Yb<sup>3+</sup> doped NLMO and (b) Kubelka- Monk plot of Pr<sup>3+</sup> doped and Pr<sup>3+</sup>/Yb<sup>3+</sup> doped NLMO.

**Figure S5.** log(I/x) Vs log(x) plot of NaLa<sub>0.97</sub>Pr<sub>0.03</sub>(MoO<sub>4</sub>)<sub>2</sub> (0.01 ≤ x ≤ 0.11).

#### Tables

**Table S1.** Rietveld refined lattice parameters and unit cell volume for NaLa<sub>1-x</sub>Pr<sub>x</sub>(MoO<sub>4</sub>)<sub>2</sub> (0.00 ≤ x ≤ 0.11) compounds.

**Table S2.** Rietveld refined structural parameters for NaLa<sub>0.97</sub>Pr<sub>0.03</sub>(MoO<sub>4</sub>)<sub>2</sub> compounds.

**Table S3.** Rietveld refined structural parameters for NaLa<sub>0.94</sub>Pr<sub>0.03</sub>Yb<sub>0.03</sub>(MoO<sub>4</sub>)<sub>2</sub> compounds.

**Table S4.** Variations of decay time ( $\tau$ ), energy transfer efficiency ( $\eta_{ETE}$ ), and quantum cutting efficiency ( $\eta_{QE}$ ) in  $\text{Pr}^{3+}/\text{Yb}^{3+}$  codoped NLMO samples on fixing the amount of  $\text{Pr}^{3+}$  and varying the amount of  $\text{Yb}^{3+}$  for the emission band 647 nm under 449 nm excitation.

### Tables

**Table S1.** Rietveld refined lattice parameters and unit cell volume for  $\text{NaLa}_{1-x}\text{Pr}_x(\text{MoO}_4)_2$  ( $0.00 \leq x \leq 0.11$ ) compounds.

Compounds	Lattice parameters (Å)		Cell volume (Å <sup>3</sup> )
	<i>a</i>	<i>c</i>	
$\text{NaLa}(\text{MoO}_4)_2$	5.347(5)	11.753(1)	336.08(8)
$\text{NaLa}_{0.99}\text{Pr}_{0.01}(\text{MoO}_4)_2$	5.345(6)	11.745(8)	335.63(8)
$\text{NaLa}_{0.97}\text{Pr}_{0.03}(\text{MoO}_4)_2$	5.344(2)	11.741(3)	335.33(4)
$\text{NaLa}_{0.95}\text{Pr}_{0.05}(\text{MoO}_4)_2$	5.343(1)	11.738(5)	335.10(7)
$\text{NaLa}_{0.93}\text{Pr}_{0.07}(\text{MoO}_4)_2$	5.341(5)	11.735(7)	334.83(7)
$\text{NaLa}_{0.91}\text{Pr}_{0.09}(\text{MoO}_4)_2$	5.339(7)	11.734(8)	334.58(8)
$\text{NaLa}_{0.89}\text{Pr}_{0.11}(\text{MoO}_4)_2$	5.339(6)	11.735(5)	334.66(4)

**Table S2.** Rietveld refined structural parameters for  $\text{NaLa}_{0.97}\text{Pr}_{0.03}(\text{MoO}_4)_2$  compounds.

Atoms	Oxidation State	Wyckoff Notation	Positional parameters			$B_{\text{iso}}$	Occupancy
			<i>x</i>	<i>y</i>	<i>z</i>		
Na	+1	4b	0.0000	0.2500	0.6250	0.500	1
La/Pr	+3	4b	0.0000	0.2500	0.6250	0.500	0.97/0.03
Mo	+6	4a	0.0000	0.2500	0.1250	0.500	2
O	-2	16f	0.7674(7)	0.1122(4)	0.0426(2)	0.500	8

Crystal system = Tetragonal, Space group =  $I41/a$  (88),

Lattice parameters,  $a = 5.344(2)$  Å,  $c = 11.741(3)$  Å, Unit cell volume =  $335.33(4)$  Å<sup>3</sup>,

$R_{\text{Factors}}$ ;  $R_p = 3.06$ ,  $R_{\text{wp}} = 4.11$ ,  $R_{\text{exp}} = 2.33$ ,  $\chi^2 = 3.11$ ,  $R_{\text{Bragg}} = 6.90$ ,  $R_F = 6.99$ .

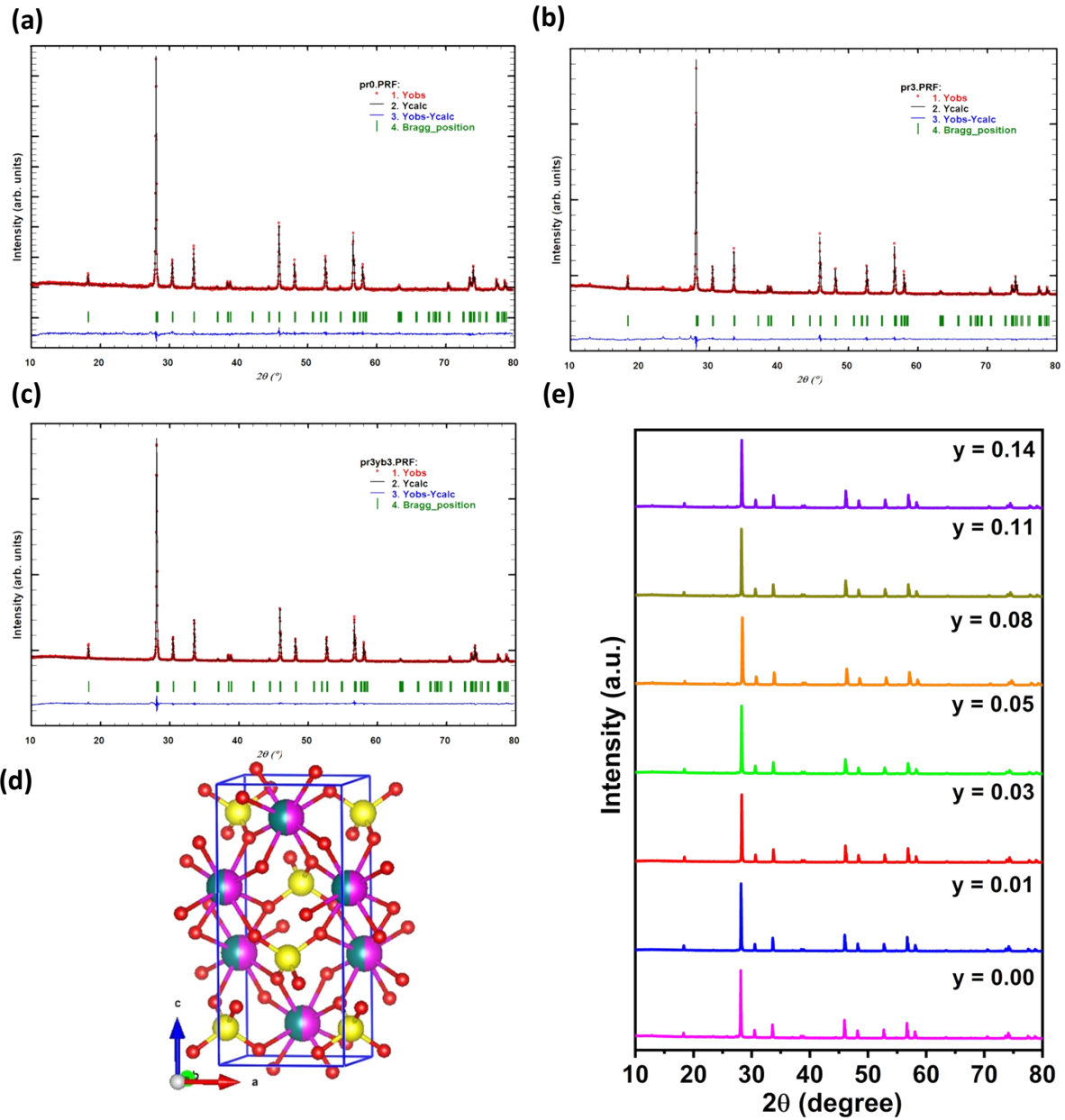
**Table S3.** Rietveld refined structural parameters for NaLa<sub>0.94</sub>Pr<sub>0.03</sub>Yb<sub>0.03</sub>(MoO<sub>4</sub>)<sub>2</sub> compounds.

Atoms	Oxidation State	Wyckoff Notation	Positional parameters			$B_{\text{iso}}$	Occupancy
			$x$	$y$	$z$		
Na	+1	4b	0.0000	0.2500	0.6250	0.500	1
La/Pr/Yb	+3	4b	0.0000	0.2500	0.6250	0.500	0.94/0.03/0.03
Mo	+6	4a	0.0000	0.2500	0.1250	0.500	2
O	-2	16f	0.7749(3)	0.1154(7)	0.0427(8)	0.500	8

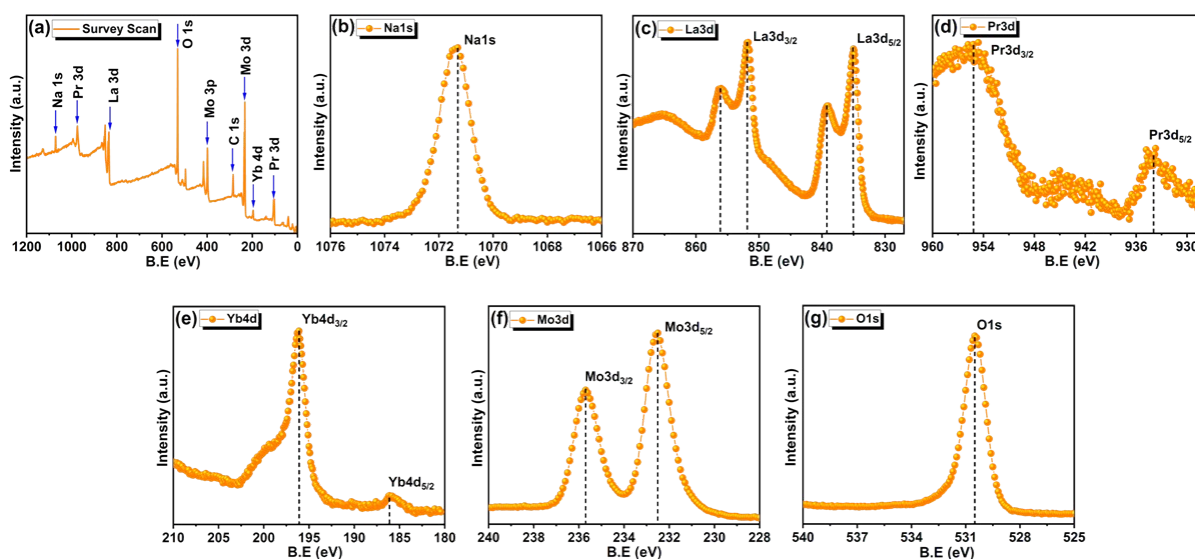
Crystal system = Tetragonal, Space group =  $I41/a$  (88),

Lattice parameters,  $a = 5.340(9)$  Å,  $c = 11.733(4)$  Å, Unit cell volume =  $334.71(2)$  Å<sup>3</sup>,

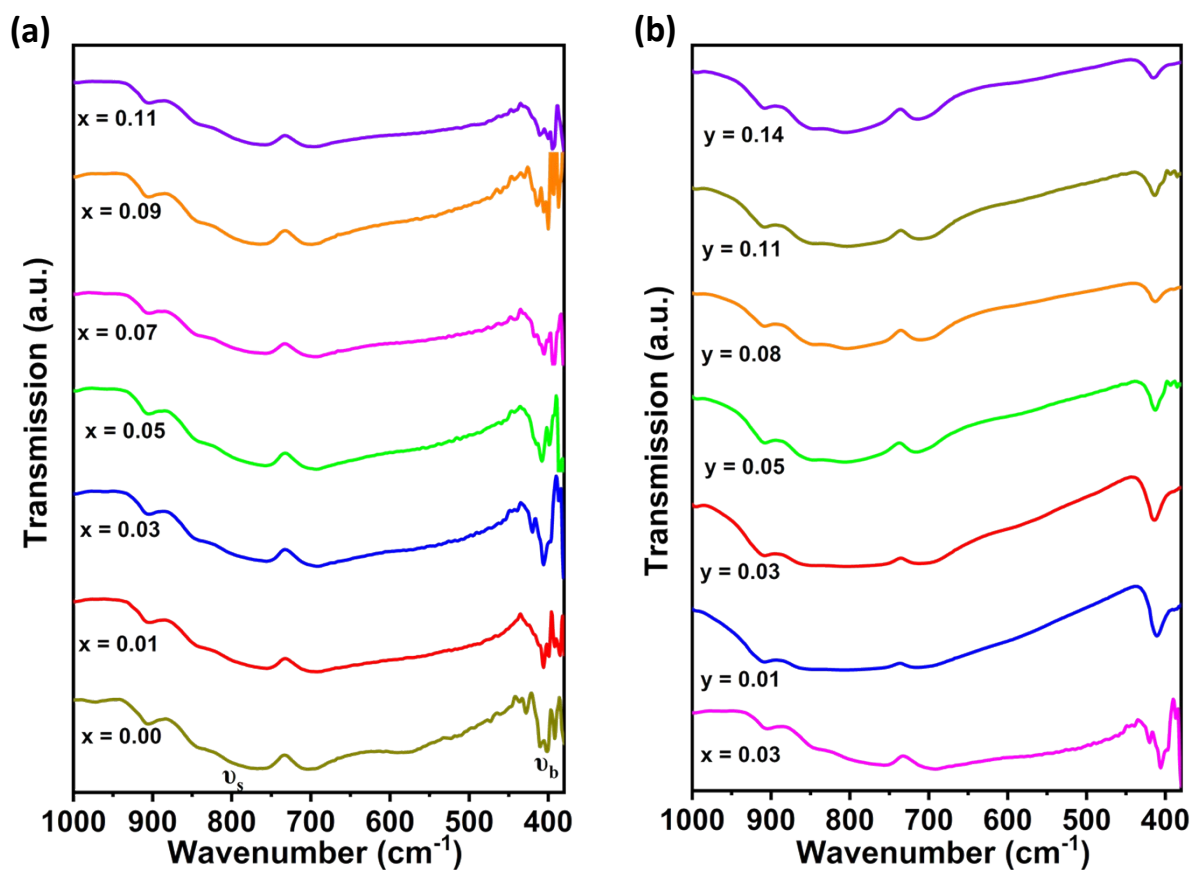
$R_{\text{Factors}}$ ;  $R_{\text{p}} = 4.61$ ,  $R_{\text{wp}} = 5.98$ ,  $R_{\text{exp}} = 4.16$ ,  $\chi^2 = 2.07$ ,  $R_{\text{Bragg}} = 3.77$ ,  $R_{\text{F}} = 7.03$ .



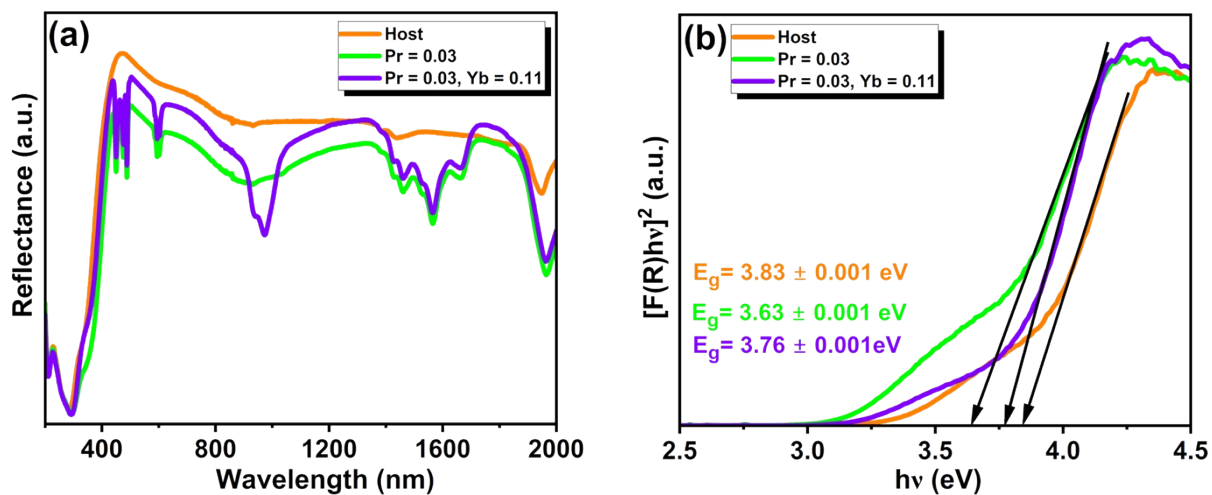
**Figure S1.** Rietveld plot of (a)  $\text{NaLa}(\text{MoO}_4)_2$ , (b)  $\text{NaLa}_{0.97}\text{Pr}_{0.03}(\text{MoO}_4)_2$  and (c)  $\text{NaLa}_{0.94}\text{Pr}_{0.03}\text{Yb}_{0.03}(\text{MoO}_4)_2$ , (d) crystal structure of  $\text{NaLa}_{0.97}\text{Pr}_{0.03}(\text{MoO}_4)_2$  and (e) XRD patterns of  $\text{NaLa}_{0.97-y}\text{Pr}_{0.03}\text{Yb}_y(\text{MoO}_4)_2$  ( $0.00 \leq y \leq 0.14$ ) phosphors.



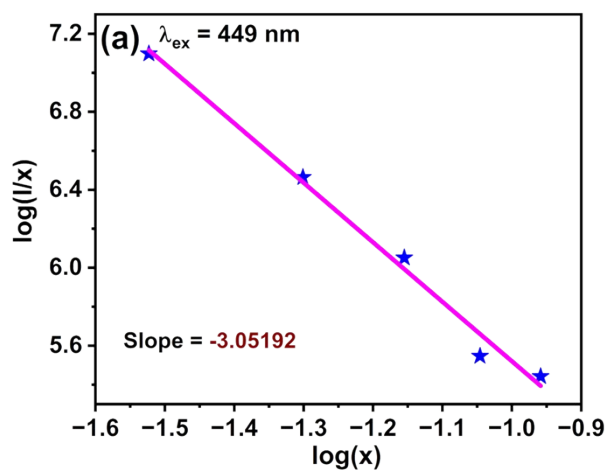
**Figure S2.** High-resolution XPS spectra of  $\text{NaLa}_{0.92}\text{Pr}_{0.03}\text{Yb}_{0.05}(\text{MoO}_4)_2$ : (a) XPS scan Survey (b) Na 1s spectra (c) La 3d spectra (d) Pr 3d, (e) Yb 4d, (f) Mo 3d spectra and (g) O 1s spectra.



**Figure S3.** FTIR spectra of  $\text{NaLa}_{1-x}\text{Pr}_x(\text{MoO}_4)_2$  and  $\text{NaLa}_{0.97-y}\text{Pr}_{0.03}\text{Yb}_y(\text{MoO}_4)_2$  phosphors.



**Figure S4.** (a) Diffusion reflectance spectra of pure,  $\text{Pr}^{3+}$  doped and  $\text{Pr}^{3+}/\text{Yb}^{3+}$  doped NLMO and (b) Kubelka- Monk plot of  $\text{Pr}^{3+}$  doped and  $\text{Pr}^{3+}/\text{Yb}^{3+}$  doped NLMO.



**Figure S5.**  $\log(I/x)$  Vs  $\log(x)$  plot of  $\text{NaLa}_{0.97}\text{Pr}_{0.03}(\text{MoO}_4)_2$  ( $0.01 \leq x \leq 0.11$ ).

**Table S4.** Variations of decay time ( $\tau$ ), energy transfer efficiency ( $\eta_{ETE}$ ), and quantum cutting efficiency ( $\eta_{QE}$ ) in Pr<sup>3+</sup>/Yb<sup>3+</sup> codoped NLMO samples on fixing the amount of Pr<sup>3+</sup> and varying the amount of Yb<sup>3+</sup> for the emission band 647 nm under 449 nm excitation.

Sample	$\tau$ ( $\mu$ S)	$\eta_{ETE}$ (%)	$\eta_{QE}$ (%)
NaLa <sub>0.97</sub> Pr <sub>0.03</sub> (MoO <sub>4</sub> ) <sub>2</sub>	6.52	-	100
NaLa <sub>0.96</sub> Pr <sub>0.03</sub> Yb <sub>0.01</sub> (MoO <sub>4</sub> ) <sub>2</sub>	6.40	1.80	102
NaLa <sub>0.94</sub> Pr <sub>0.03</sub> Yb <sub>0.03</sub> (MoO <sub>4</sub> ) <sub>2</sub>	6.38	2.14	103
NaLa <sub>0.92</sub> Pr <sub>0.03</sub> Yb <sub>0.05</sub> (MoO <sub>4</sub> ) <sub>2</sub>	6.33	2.91	104
NaLa <sub>0.89</sub> Pr <sub>0.03</sub> Yb <sub>0.08</sub> (MoO <sub>4</sub> ) <sub>2</sub>	6.17	5.36	106
NaLa <sub>0.86</sub> Pr <sub>0.03</sub> Yb <sub>0.11</sub> (MoO <sub>4</sub> ) <sub>2</sub>	6.01	7.82	108
NaLa <sub>0.83</sub> Pr <sub>0.03</sub> Yb <sub>0.14</sub> (MoO <sub>4</sub> ) <sub>2</sub>	5.96	8.58	109