Electronic Supplementary Information

Microwave-Assisted Solid-State Synthesis of $NaRE(MO_4)_2$ Phosphors (RE = La, Pr, Eu, Dy; M = Mo, W)

S. Sameera Perera,[⊥] Hashini N. Munasinghe,[⊥] Emily N. Yatooma, and Federico A. Rabuffetti[*]

Department of Chemistry, Wayne State University, Detroit, MI 48202, USA

[⊥]These authors contributed equally

*Corresponding Author. Email: far@chem.wayne.edu

Table S1. Structural Parameters of Na_2MO_4 and $NaRE(MO_4)_2$

	Na_2MO_4		$NaEu(MO_4)_2$		$NaLa_{0.95}Eu_{0.05}(MO_4)_2$		$NaLa_{0.95}Pr_{0.025}Dy_{0.025}(MO_4)_2$	
M	Mo	W	Mo	W	Mo	W	Mo	W
a (Å)	9.10985(10)	9.12938(12)	5.24577(8)	5.25722(8)	5.33755(6)	5.35498(5)	5.33988(3)	5.34993(5)
c (Å)	–	–	11.4682(2)	11.4079(2)	11.71844(19)	11.65403(13)	11.72515(8)	11.64530(17)
V (Å^3)	756.02(3)	760.90(3)	315.582(12)	315.296(12)	333.852(10)	334.189(8)	334.334(5)	333.309(9)
xO	0.26172(14)	0.2582(4)	0.1426(13)	0.1470(15)	0.1389(11)	0.1441(13)	0.1334(6)	0.1432(18)
yO	0.26172(14)	0.2582(4)	0.4663(12)	0.4721(12)	0.4744(9)	0.4790(11)	0.4847(6)	0.4763(14)
zO	0.26172(14)	0.2582(4)	0.2065(5)	0.2087(6)	0.2073(4)	0.2069(5)	0.2051(3)	0.2029(7)
$U_{iso}^{Na/RE}$	0.46(4)	0.10	1.34(6)	2.45(9)	1.84(12)	0.73(8)	0.30	1.07(5)
U_{iso}^{M}	0.45(4)	0.10	1.34(6)	1.20(5)	0.48(8)	1.61(5)	0.30	1.07(5)
U_{iso}^{O}	1.50(10)	0.15	0.6(3)	1.0(4)	3.0(3)	1.8(3)	0.45	2.9(4)
R_{wp} (%)	5.5	10.0	5.8	6.4	8.0	8.4	7.0	9.6

U_{iso} values given as $100 \times U$.

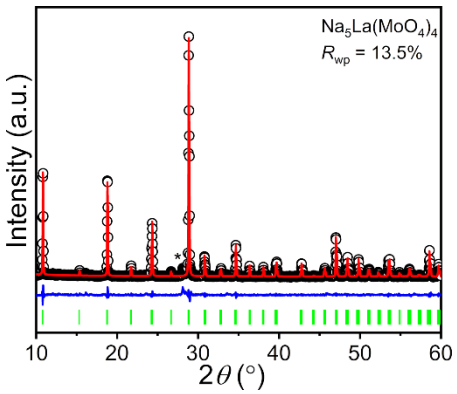

Figure S1. Rietveld analysis of the PXRD pattern of the quadruple molybdate $Na_5La(MoO_4)_4$ (PDF No. 01–072–2158) obtained via microwave-assisted solid-state reaction (sample mass: 0.20 g; power: 600 W; heating profile: 9 cycles of 3 min each; total time: 27 min). Experimental data (○), calculated pattern (—), and difference curve (—, offset for clarity) are shown. Tick marks (|) corresponding to the calculated position of the diffraction maxima are included. The peak depicted with a * symbol corresponds to the double molybdate $NaLa(MoO_4)_2$, which appears as a secondary phase.

Table S2. Structural Parameters of $Na_5La(MoO_4)_4$

	x	*y*	*z*	U_{iso}
Na1	0.0	0.25	0.625	0.7(3)
La1	0.0	0.25	0.125	0.7(3)
Na2	0.1270(18)	0.042(2)	0.3392(14)	0.7(3)
Mo1	0.1784(5)	0.3474(9)	0.3923(4)	1.8(3)
O1	0.168(3)	0.459(3)	0.484(3)	1.1(5)
O2	0.149(3)	0.221(3)	0.475(3)	1.1(5)
O3	0.058(3)	0.367(3)	0.295(3)	1.1(5)
O4	0.317(3)	0.332(3)	0.318(2)	1.1(5)

$Na_5La(MoO_4)_4$: space group $I4_1/a$, a = 11.5750(2) Å, c = 11.6210(3) Å, V = 1556.99(8) Å^3.
U_{iso} values given as 100 × U.

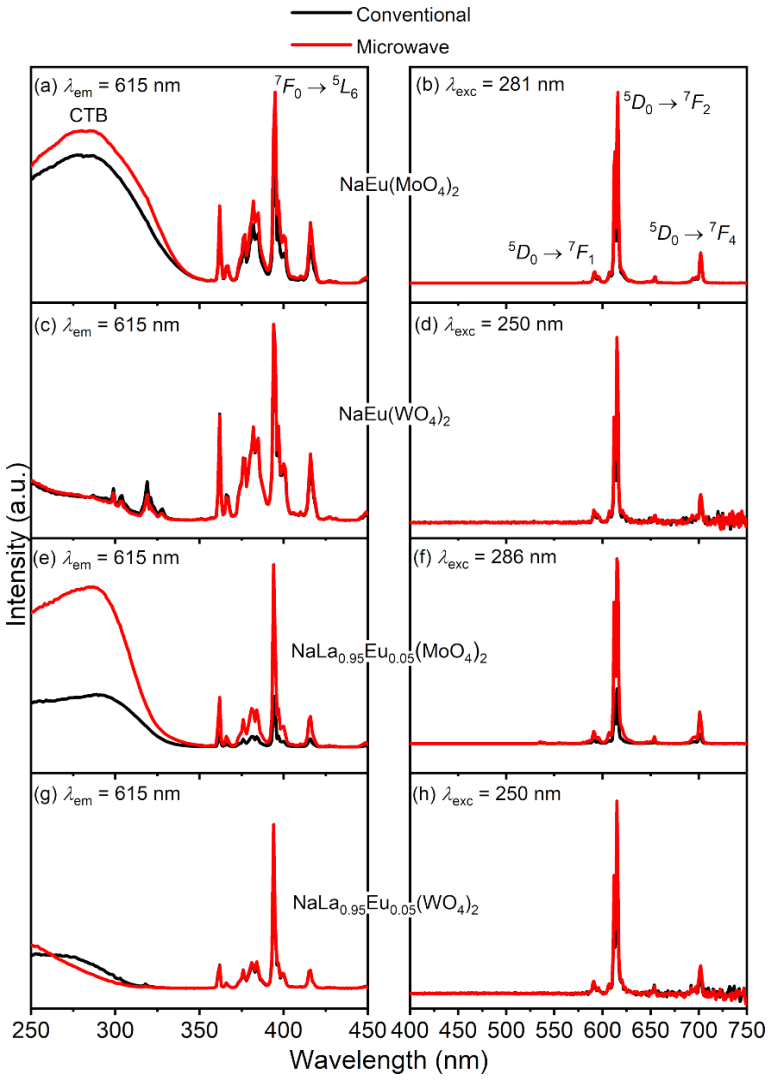

Figure S2. Excitation and emission spectra of Eu^{3+}-containing metalate phosphors synthesized using conventional and microwave heating. Metal-to-oxygen charge-transfer band (CTB) and selected f–f transitions of Eu^{3+} are indicated in (a) and (b).