Supplementary information for:

Determination of Crystal Structure and Photoluminescence Properties of $NaEu_{1-x}Gd_x(MoO_4)_2$ Phosphor Synthesised by Water-Assisted Low-Temperature Synthesis Technique

Takuya Hasegawa,[a,†] Sun Woog Kim,*[a,‡] Yusuke Abe,[a] Masaru Muto,[a] Mizuki Watanabe,[a] Tatsuro Kaneko,[a] Kazuyoshi Uematsu,[a] Tadashi Ishigaki,[a] Kenji Toda,*[a] Mineo Sato,[d] Junko Koide,[e] Masako Toda[e] and Yoshiaki Kudo[e]

[a]*Graduate School of Science and Technology, Niigata University, 8050 Ikarashi 2-nocho, Niigata, 950-2181, Japan.*
[b]*Department of Chemistry and Chemical Engineering, Niigata University, 8050 Ikarashi 2-nocho, Niigata 950-2181, Japan.*
[c]*N-Luminescence Corporation, 8867-3 Ikarashi 2-nocho, Niigata 950-2101, Japan.*
[†]*Current address: Department of Marine Resource Science, Faculty of Agriculture and Marine Science, Kochi University, 200 Otsu, Monobe, Nankoku City, Kochi 783-8502, Japan.*
[‡]*Current address: Department of Nanotechnology and Advanced Material Engineering, Sejong University, 209 Neungdong-ro, Gwangjin-gu, Seoul 05006, Republic of Korea.*

Corresponding author:
S.W. Kim; skim80@sejong.ac.kr
K. Toda; ktoda@eng.niigata-u.ac.jp

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Table S1. Synthesis of $RbVO_3$ phosphor by the WASSR method as a function of solvents

Synthesis conditions of $RbVO_3$			
Raw materials	Rb_2CO_3, V_2O_5		
Solvent	10 wt% for the obtained material		
Mixing time	3 min.		
Solvent	Obtained material	Solvent	Obtained material
de-ionized water	$RbVO_3$	chloroform	Rb_2CO_3, V_2O_5
ethanol (95%)	$RbVO_3$, Rb_2CO_3, V_2O_5	acetylacetone	Rb_2CO_3, V_2O_5
ethanol (dehydration)	Rb_2CO_3, V_2O_5	tetrahydrofuran (dehydration)	Rb_2CO_3, V_2O_5
hydrogen peroxide	Rb_2CO_3, V_2O_5	2-butanone	Rb_2CO_3, V_2O_5
methanol	Rb_2CO_3, V_2O_5	cyclohexane	Rb_2CO_3, V_2O_5
acetone	Rb_2CO_3, V_2O_5	toluene	Rb_2CO_3, V_2O_5
hexanol	Rb_2CO_3, V_2O_5	xylene	Rb_2CO_3, V_2O_5
1-butanol	Rb_2CO_3, V_2O_5	1,1,1-trichloroethane	Rb_2CO_3, V_2O_5
n- pentyl alcohol	Rb_2CO_3, V_2O_5	tetrachloroethylene	Rb_2CO_3, V_2O_5
3-methyl-1-butanol	Rb_2CO_3, V_2O_5	chlorobenzene	Rb_2CO_3, V_2O_5
2-methoxyethanol	Rb_2CO_3, V_2O_5	octylphenol ethoxylate	Rb_2CO_3, V_2O_5
benzyl alcohol	Rb_2CO_3, V_2O_5	ligroin	Rb_2CO_3, V_2O_5
ethylene glycol	Rb_2CO_3, V_2O_5	bis(2-ethylhexyl)phthalate	Rb_2CO_3, V_2O_5
propylene glycol	Rb_2CO_3, V_2O_5	dimethyl carbonate	Rb_2CO_3, V_2O_5
1,4-butanediol	Rb_2CO_3, V_2O_5	propylene carbonate	Rb_2CO_3, V_2O_5
diethylene glycol	Rb_2CO_3, V_2O_5	formic acid	Rb_2CO_3, V_2O_5
polyethylene glycol	Rb_2CO_3, V_2O_5	oleic acid	Rb_2CO_3, V_2O_5
1-amino-2-propanol	Rb_2CO_3, V_2O_5	phosphoric acid	Rb_2CO_3, V_2O_5
2,2'-iminodimethanol	Rb_2CO_3, V_2O_5		

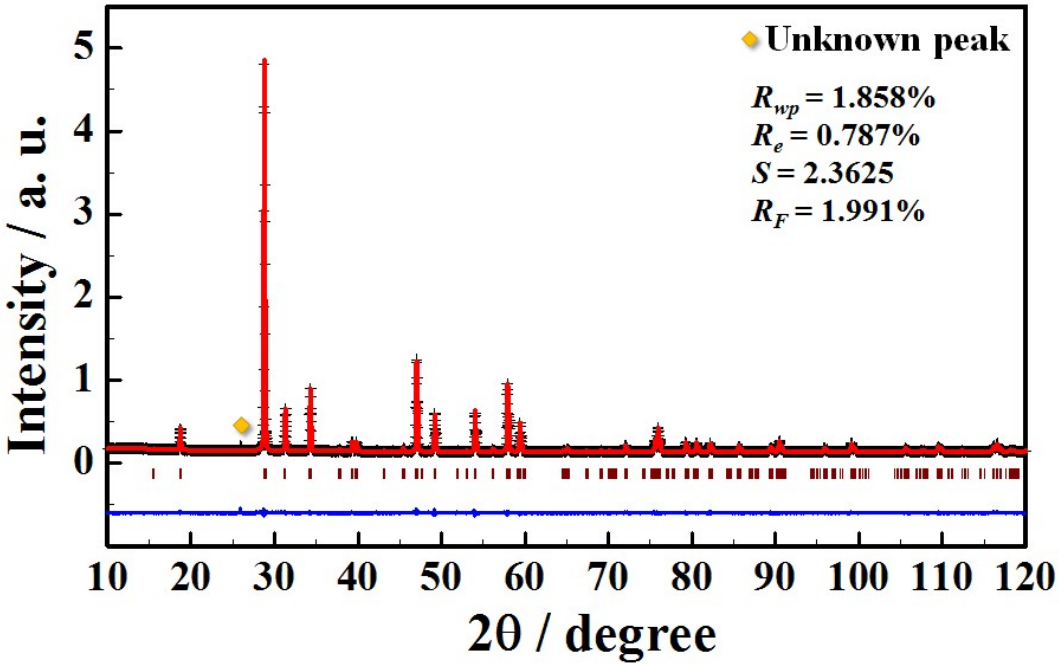

Figure S1. Observed (+) and calculated (red line) X-ray powder diffraction data of $NaEu(MoO_4)_2$ phosphor prepared by the conventional SSR method as well as the difference profile (blue bottom line) between them. Bragg reflection peak positions are shown as vertical bars. Inset shows the R-factors and S value of this refinement.

Table S2. Refined structural parameters of $NaEu(MoO_4)_2$ phosphor prepared by the conventional SSR method.

$NaEu(MoO_4)_2$						
Atom	Site	Occupancy	*x*	*y*	*z*	U_{iso} (nm^2)
Na1	4e	0.485(3)	1/2	0	0.1248(7)	0.0088(5)
Eu1	4e	0.5149	1/2	0	0.1248	0.00877
Mo1	4e	1	1/2	0	0.6247(5)	0.0067(3)
O1	8f	1	0.637(2)	0.136(2)	0.3010(7)	0.015(1)
O2	8f	1	0.267(2)	0.232(2)	0.0357(6)	0.01548

Because of the disordering of Eu and Na atoms, the fractional coordinate and atomic displacement parameters (U_{iso}) were constraint to the same values, respectively.

Table S3. Bond distances between metal and oxygen in the $NaEu(MoO_4)_2$ nano phosphor prepared by WASSR method.

	WASSR method	SSR method
Metal-oxygen bonding	Bond distance (nm)	Bond distance (nm)
Eu1/Na1-O1	0.262(1) × 2	0.263(1) × 2
Eu1/Na1-O1	0.2688(6) × 2	0.2592(8) × 2
Eu1/Na1-O2	0.230(1) × 2	0.238(1) × 2
Eu1/Na1-O2	0.2345(6) × 2	0.2366(9) × 2
Mo1-O1	0.1537(8) × 2	0.155(1) × 2
Mo1-O2	0.198(1) × 2	0.193(1) × 2

3. Explanation for the treatment of crystallographic data

3.1. Transformation of Space group No. 15

The standard expression of No. 15 is "*C* 1 2/*c* 1", sometimes abbreviated as "*C*2/*c*". The structure parameters of $NaEu(MoO_4)_2$ have already been refined based on the non-standard *I* 1 1 2/*b* (*I*2/*b*).[2] The International Union of Crystallography (IUCr) recommends the usage of standard expression of space group. In *I* 1 1 2/*b* space group, the unique axis is *c* axis, not recommended either, formally b axis in monoclinic system. So, we decided the refinement for our sample to be based on the standard *C* 1 2/*c* 1.

The relationship of axes between *C* 1 2/*c* 1 and *I* 1 1 2/*b* is shown in **Figure S2**. The subscript letters correspond to Bravais lattices, *C* and *I*. The basic vectors, $\boldsymbol{c}_I$ and $\boldsymbol{b}_c$, are perpendicular to the paper.

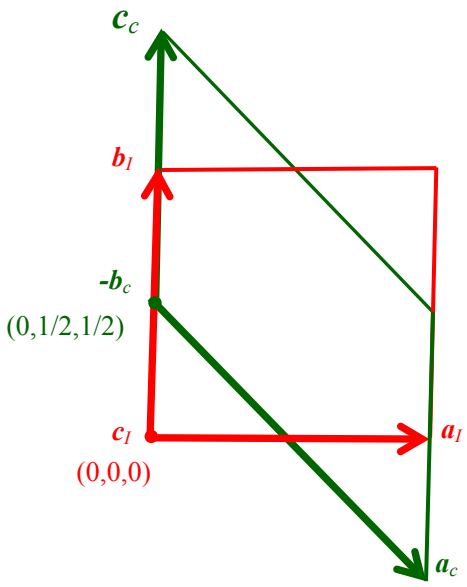

Figure S2. Relationship of axes between *C* 1 2/*c* 1 and *I* 1 1 2/*b*

The origin of *C* lattice should be moved on (0,1/2,1/2), this being because of the transformation from *I* to *C*.[1] The linear combinations between these vectors can be expressed as follows;

$a_c = a_I - b_I$

$b_c = -c_I$

$c_c = b_I$

and

$$t = \frac{1}{2}b_I + \frac{1}{2}c_I$$

where t is the translational vector of origin. By means of matrices and vectors, we can

express these equations to the following equation.

$$\begin{pmatrix} a_C \\ b_C \\ c_C \end{pmatrix} = Q \begin{pmatrix} a_I \\ b_I \\ c_I \end{pmatrix} + t \qquad (1)$$

where

$$Q = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} and\ t = \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \end{pmatrix}$$

We can also an inverse relation like

$$\begin{pmatrix} a_I \\ b_I \\ c_I \end{pmatrix} = Q^{-1} \begin{pmatrix} a_C \\ b_C \\ c_C \end{pmatrix} - t \qquad (2)$$

where

$$Q^{-1} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}$$

The atomic coordinates, (x_i,y_i,z_i), can be transformed by the following equation.

$$\begin{pmatrix} x_C \\ y_C \\ z_C \end{pmatrix} = R \begin{pmatrix} x_I \\ y_I \\ z_I \end{pmatrix} - Rt \qquad (3)$$

where

$$R = Q^{t\,-1}$$

and Q^t means transposed matrix of $\boldsymbol{Q}$.

3.2. Rietveld refinement based on *C* 1 2/*c* 1

Using above equations (1) and (3), the reported crystallographic data[2] were transformed to the data on *C* 1 2/*c* and taken as initial refined parameters for Rietveld analysis. Treatment of the XRD patterns was carried out using the Rietan-FP program.[3] Because of the disordering of Eu and Na atoms, the fractional coordinate and atomic displacement parameters (U_{iso}) were constraint to the same values, respectively. In the early stage of refinement, the values of U_{iso} for two oxygen atoms, O1 and O2, were converged to too much different values in spite of the fact that the two atoms have similar crystallographic environment. This is because the oxygen atoms are of much less atomic number compared heavy Eu and Mo in $NaEu(MoO_4)_2$, making their U_{iso}'s less reliable. Therefore, the U_{iso} values were constraint to be same. Finally, the refinement was converged to an excellent fitting, having *R* factors; R_{wp}=1.690%, R_p=1.139%, R_R=10.335%, R_e=0.737%, S=2.2936, R_B=3.567%, R_F=2.816% and

R_{F^2}=3.876.

Table S4 shows the results based on *C* 1 2/*c* 1. Using the equation (2), the data were transformed back to the data on *I* 1 1 2/*b*, making the data easily compared with those previously reported[2]. Table S5 and Table S6 on *C* 1 2/*c* 1 are our data and the reported data, respectively.

Table S4. Structural parameters of $NaEu(MoO_4)_2$ refined on space group *C* 1 2/*c* 1. SG=*C* 1 2/*c* 1, *a*=0.74214(6) nm, *b*=1.14644(1) nm, *c*=0.52475(4) nm, *β*=134.999(4) º, *V*=0.31570(4) nm^3

Atom	site	*g*	*x*	*y*	*z*	U_{iso}
Eu1	4e	0.504(3)	0	0.1210(4)	1/4	0.0094(5)
Na1	4e	0.4961	0	0.12096	1/4	0.00943
Mo1	4e	1	0	0.6266(3)	1/4	0.0076(4)
O1	8f	1	0.127(1)	0.2950(6)	0.077(2)	0.013(1)
O2	8f	1	0.224(2)	0.0381(5)	0.143(2)	0.01271

Table S5. Structural parameters transformed from space group *C* 1 2/*c* 1 to space group *I* 1 1 2/*b*. SG=*I* 1 1 2/*b*, *a*=0.52478 nm, *b*=0.52475 nm, *c*=1.14644 nm, *γ*=89.9992 º, *V*=0. 31570 nm^3

Atom	site	*g*	*x*	*y*	*z*	U_{iso}
Eu1	4e	0.5039	0	1/4	0.1210	0.0094(5)
Na1	4e	0.4961	0	1/4	0.1210	0.00943
Mo1	4e	1	0	1/4	0.6266	0.0076(4)
O1	8f	1	0.8730	0. 9496	0.2950	0.013(1)
O2	8f	1	0.7764	0.9194	0.0380	0.01271

Table S6. Structural parameters of $NaEu(MoO_4)_2$ reported[2] . SG=*I* 1 1 2/*b*, *a*=0.52421(1) nm, *b*=0.52385(1) nm, *c*=1.14543(2) nm, *γ*=89.949(3) º , *V*=0.31454 nm^3

Atom	site	*g*	*x*	*y*	*z*	U_{iso}
Eu1	4e	0.5	1/2	1/4	0.8758(4)	0.0077(5)
Na1	4e	0.5	1/2	1/4	0.8758(4)	0.0077(5)
Mo1	4e	1	1/2	1/4	0.3738(4)	0.0097(5)
O1	8f	1	0.373(1)	0.016(2)	0.2810(7)	0.0017(8)
O2	8f	1	0.749(2)	0.434(1)	0.0478(6)	0.0017(8)

Table S7. Refinement and cell parameters of the $NaEu_{1-x}Gd_x(MoO_4)_2$ (x = 0 and 0.30) phosphors.

	$NaEu(MoO_4)_2$	$Na(Eu_{0.70}Gd_{0.30})(MoO_4)_2$
Crystal system	monoclinic	monoclinic
Space group	*C*2/*c*	*C*2/*c*
a (nm)	0.74214(6)	0.7412(4)
b (nm)	1.14644(1)	1.14694(8)
c (nm)	0.52475(4)	0.5241(3)
β (°)	134.999(4)	135.00(3)
V (nm^3)	0.31570(4)	0.3150(3)

References

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2. A. Arakcheeva, D. Logvinovich, G. Chapuis, V. Morozov, S. V. Eliseeva, J. C. G. Bünzli and P. Pattison, *Chem. Sci*., 2012, **3**, 384.

3. F. Izumi and K. Momma, *Solid State Phenom.*, 2007, **130**, 15