Supporting Information

Crystal Structure Elucidation and Luminescent Properties of Blue-Emitting $BaMgSi_3O_8:Eu^{2+}$ Phosphor with Alkali Feldspar Structure

Wataru Hikita[†], Mineo Sato[‡] and Kenji Toda[†,*]

† Graduate School of Science and Technology, Niigata University, 8050 Ikarashi 2-nocho, Niigata 950-2181, Japan

‡ Department of Chemistry and Chemical Engineering, Faculty of Engineering, Niigata University, 8050 Ikarashi 2-nocho, Niigata 950-2181, Japan

***Corresponding Author**

Kenji Toda

E-mail: ktoda@eng.niigata-u.ac.jp

TEL/FAX: 025-262-6771

Table S1 Lattice parameters and crystallographic data of $BaMgSi_3O_8$ phase in the $BaMgSi_4O_{10}$:Eu^{2+} compositional powder refined by the Rietveld analysis.

Chemical formula			$BaMgSi_3O_8$			
Space group			$P\bar{1}$ (#64)			
a [Å]			7.2760(8)			
b [Å]			7.5686(10)			
c [Å]			8.2003(10)			
α [°]			113.351(7)			
β [°]			103.549(6)			
γ [°]			102.951(7)			
V [Å^3]			376.79(9)			
Atom	Wyckoff positions	Occupancy	*x*	*y*	*z*	B_{eq}
Ba1	2i	1	0.8702(4)	0.2082(4)	0.2382(4)	1.07(9)
Si1	2i	1	0.329(2)	0.083(2)	0.330(2)	0.5(3)
Si2	2i	1	0.364(2)	0.304(2)	0.091(1)	0.4(3)
Si3	2i	1	0.249(1)	0.680(2)	0.333(2)	0.6(3)
Mg1	2i	1	0.204(2)	0.312(2)	0.705(2)	1.9(4)
O1	2i	1	0.032(3)	0.636(3)	0.377(3)	0.5
O2	2i	1	0.295(3)	0.115(3)	0.140(3)	0.9(6)
O3	2i	1	0.200(2)	0.159(3)	0.433(3)	0.5
O4	2i	1	0.275(3)	0.460(3)	0.205(3)	1.1(6)
O5	2i	1	0.608(3)	0.386(3)	0.169(3)	0.6(6)
O6	2i	1	0.263(3)	0.191(3)	0.857(3)	0.6(6)
O7	2i	1	0.286(3)	0.831(3)	0.251(3)	0.5
O8	2i	1	0.569(2)	0.183(3)	0.441(3)	0.5
Phase ratio (mass%)						
$BaMgSi_3O_8$			76.51			
$BaSi_2O_5$			5.85			
SiO_2 (α-cristobalite)			15.99			
SiO_2 (α-quartz)			1.65			

Table S2 Lattice parameters and crystallographic data of $BaMgSi_3O_8$ phase in the $BaMgSi_3O_8:Eu^{2+}$ compositional powder refined by the Rietveld analysis.

Chemical formula			$BaMgSi_3O_8$			
Space group			$P\bar{1}$ (#64)			
a [Å]			7.2792(9)			
b [Å]			7.573(1)			
c [Å]			8.203(1)			
α [°]			113.302(8)			
β [°]			103.572(7)			
γ [°]			102.978(7)			
V [Å^3]			377.3(1)			
Atom	Wyckoff positions	Occupancy	*x*	*y*	*z*	B_{eq}
Ba1	2i	1	0.8695(3)	0.2090(3)	0.2377(3)	1.13(9)
Si1	2i	1	0.326(1)	0.078(2)	0.329(1)	0.3(2)
Si2	2i	1	0.365(1)	0.309(2)	0.092(1)	0.8(3)
Si3	2i	1	0.248(1)	0.677(2)	0.334(1)	1.0(2)
Mg1	2i	1	0.203(2)	0.312(2)	0.696(2)	1.5(3)
O1	2i	1	0.042(2)	0.630(2)	0.364(2)	0.5
O2	2i	1	0.293(2)	0.108(2)	0.137(2)	0.7(5)
O3	2i	1	0.202(2)	0.172(2)	0.442(2)	0.5
O4	2i	1	0.269(2)	0.460(3)	0.198(2)	1.3(5)
O5	2i	1	0.614(2)	0.395(2)	0.171(2)	0.5
O6	2i	1	0.257(2)	0.197(2)	0.860(2)	0.5
O7	2i	1	0.272(2)	0.828(3)	0.251(2)	0.5
O8	2i	1	0.572(2)	0.200(3)	0.447(2)	1.0(5)
Phase ratio (mass%)						
$BaMgSi_3O_8$			93.23			
$BaSi_2O_5$			5.39			
SiO_2 (α-cristobalite)			1.38			

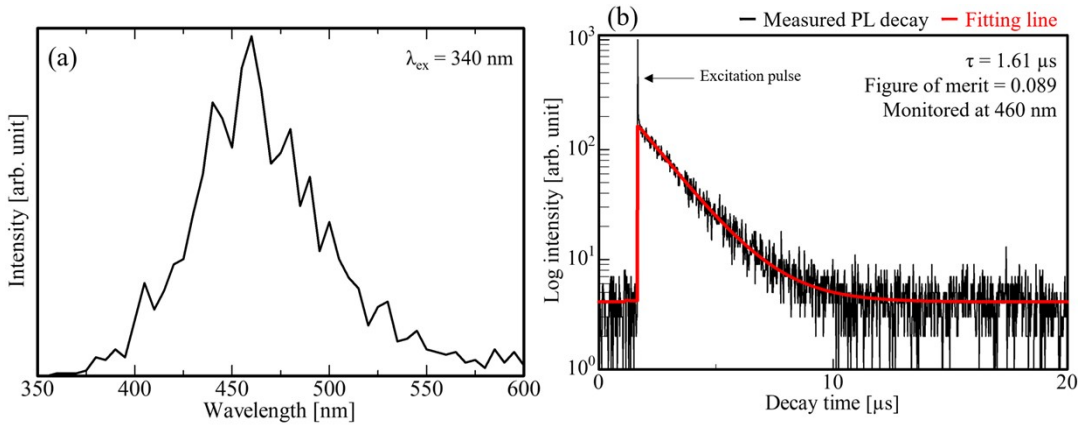

Fig. S1 (a) PL spectrum and (b) PL decay curve of blue-emitting single crystal obtained from the $BaMgSi_4O_{10}:Eu^{2+}$ compositional sample.

To compare with the luminescence properties of the powder samples, the PL spectrum and PL decay curve of the blue-emitting single crystals were measured. In the measurement of PL spectrum, sufficient emission intensity could not be detected due to the small volume of single crystal sample, but it found clearly that the peak of PL spectrum is at approximately 460 nm. The PL decay lifetime of single crystal was a single component and τ = 1.61 μs.

The PL spectra of single crystals of impurity phases cannot be measured because impurity particles did not grow to a size that can be collected as single crystal particles, and they existed in the form of small attachments on the surface of blue-emitting particles.