Electronic Supplementary Information

Stabilization of Novel High Temperature Phase Yellow-emitting σ−type $(Ba_{1-x-y}Eu_xMg_y)_2P_2O_7$ Phosphor using Melt Synthesis Technique

Hiroko Nakagawa [†,‖], Sun Woog Kim [*,†,§,‖], Takuya Hasegawa [†,¶,‖], Shota Hasegawa [†], Tadashi Ishigaki [†], Kazuyoshi Uematsu [†], Kenji Toda [*,†], Mineo Sato [‡] and Hiromitsu Takaba [#]

*Corresponding Author
Sun Woog Kim; E-mail: skim@eng.niigata-u.ac.jp
Kenji Toda; E-mail: ktoda@eng.niigata-u.ac.jp

‖These authors contributed equally.

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Table S1. Crystallographic data of σ–$Ba_2P_2O_7$, σ–$(Ba_{0.99}Eu_{0.03})_2P_2O_7$ and σ–$(Ba_{0.69}Eu_{0.03}Mg_{0.30})_2P_2O_7$ obtained from the Rietveld refinement using X-ray powder diffraction data taken at room temperature.

Crystal system	σ–$Ba_2P_2O_7$	σ–$(Ba_{0.99}Eu_{0.03})_2P_2O_7$	σ–$(Ba_{0.69}Eu_{0.03}Mg_{0.30})_2P_2O_7$
	Hexagonal	Hexagonal	Hexagonal
Space group	*P-62m* (No.189)	*P-62m* (No.189)	*P-62m* (No.189)
a (nm)	0.94168(5)	0.941292(2)	0.941292(3)
b (nm)	0.941677	0.941292	0.941292
c (nm)	0.70844(3)	0.707896(4)	0.708571(3)
V (nm)	0.54405(5)	0.54318(6)	0.54348(3)
Z	4	4	4
R_P (%)	6.371	7.547	7.424
R_{WP} (%)	8.826	10.73	10.58
R_F (%)	1.488	2.231	3.137
S	2.4101	2.3856	2.8868

Table S2. Ba-O distance of σ–$Ba_2P_2O_7$, σ–$(Ba_{0.99}Eu_{0.03})_2P_2O_7$ and σ–$(Ba_{0.69}Eu_{0.03}Mg_{0.30})_2P_2O_7$obtained from the Rietveld refinement using X-ray powder diffraction data taken at room temperature.

(Unit: nm)

	σ–$Ba_2P_2O_7$	σ–$(Ba_{0.99}Eu_{0.03})_2P_2O_7$	σ–$(Ba_{0.69}Eu_{0.03}Mg_{0.30})_2P_2O_7$
Ba1–O1 × 2	0.2749	0.2884	0.2864
Ba1–O2 × 4	0.2829	0.2834	0.2787
Ba1–O3	0.3647	0.3395	0.3652
Ba2–O1 × 4	0.2975	0.2869	0.2995
Ba2–O2 × 4	0.2893	0.2847	0.2852
Ba2-O4	0.3377	0.3497	0.3460

Table S3. P–P distances and P–O–P angles of σ−$(Ba_{0.99}Eu_{0.03})_2P_2O_7$, σ−$(Ba_{0.72}Eu_{0.03}Mg_{0.25})_2P_2O_7$ and σ−$(Ba_{0.69}Eu_{0.03}Mg_{0.30})_2P_2O_7$ obtained from the Rietveld refinement using X-ray powder diffraction data taken at room temperature.

Formula	distance of P−P (nm)		angle of P-O-P (°)	
	BaO_9	BaO_7	BaO_9	BaO_7
σ−$Ba_2P_2O_7$	0.3211	0.2871	148	100
σ−$(Ba_{0.99}Eu_{0.03})_2P_2O_7$	0.2934	0.2818	104	70
σ−$(Ba_{0.69}Eu_{0.03}Mg_{0.30})_2P_2O_7$	0.2902	0.3006	107	118

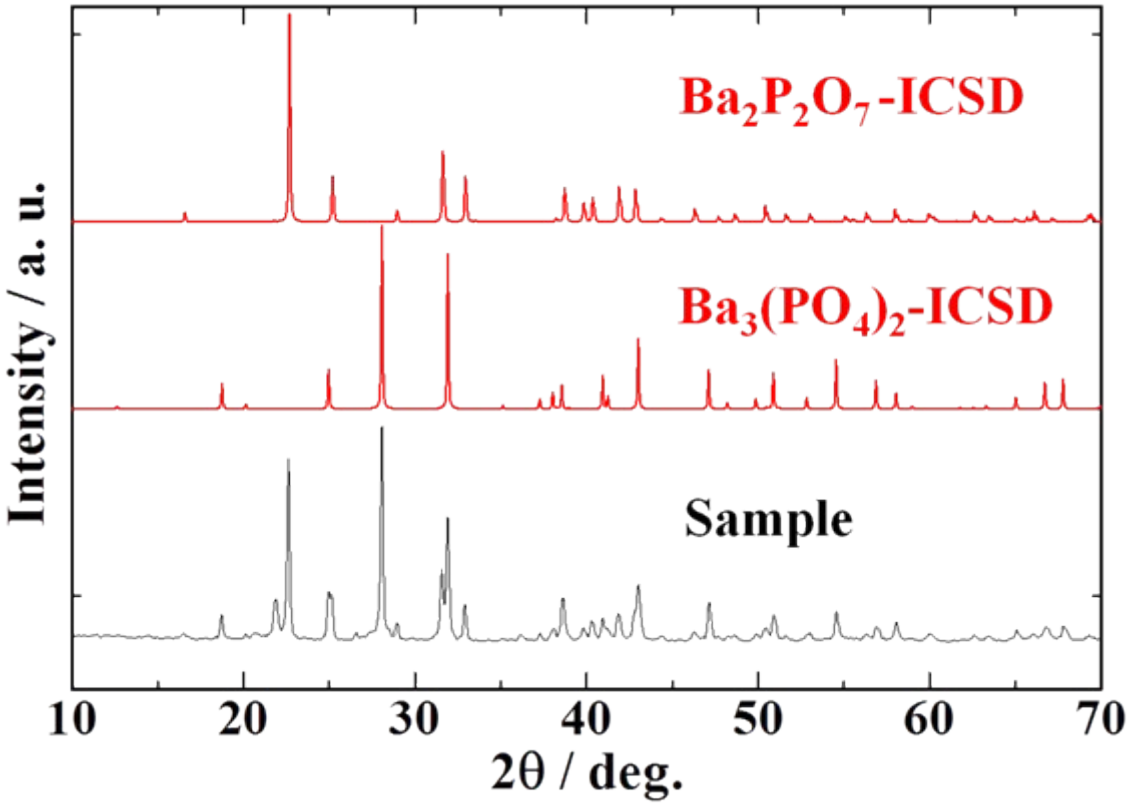

Figure S1. XRD patterns of the σ–$(Ba_{0.99}Eu_{0.03})_2P_2O_7$ phosphor synthesized by conventional solid state reaction.

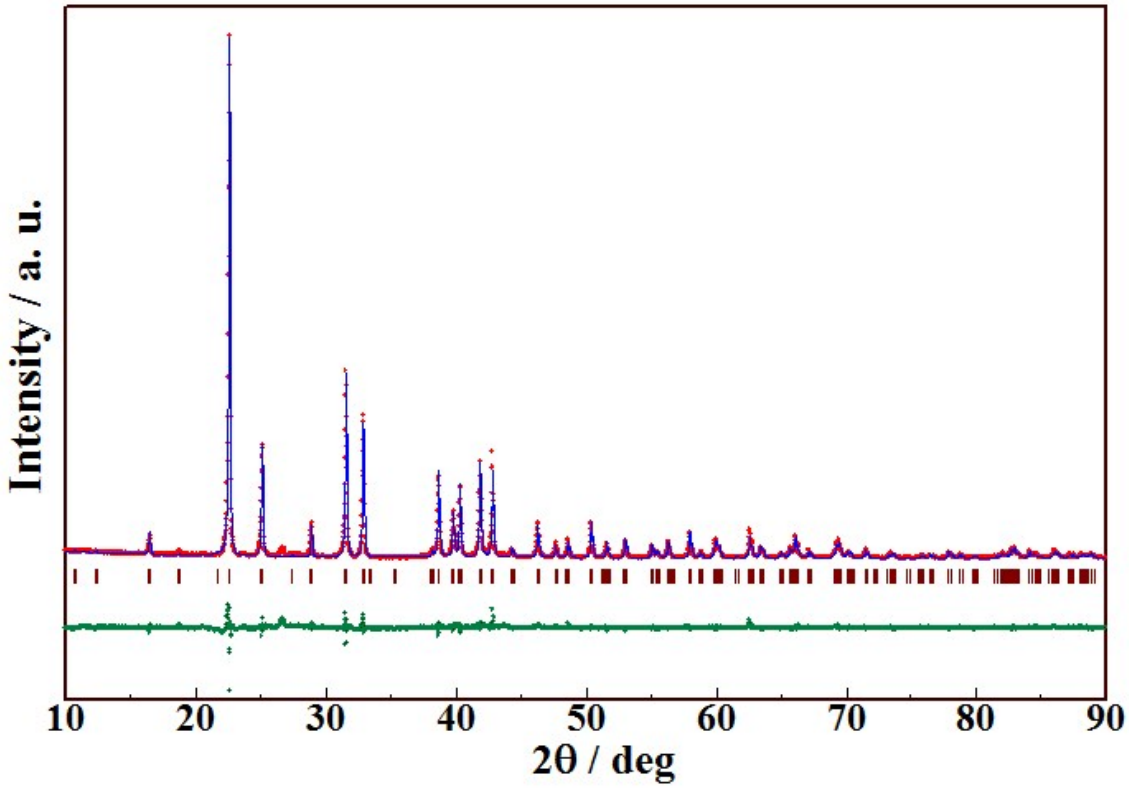

Figure S2. Observed (red + symbol), calculated (blue solid line) and difference (green solid line) patterns for the Rietveld refinement from the X-ray powder diffraction data of the synthesized σ–$(Ba_{0.97}Eu_{0.03})_2P_2O_7$.

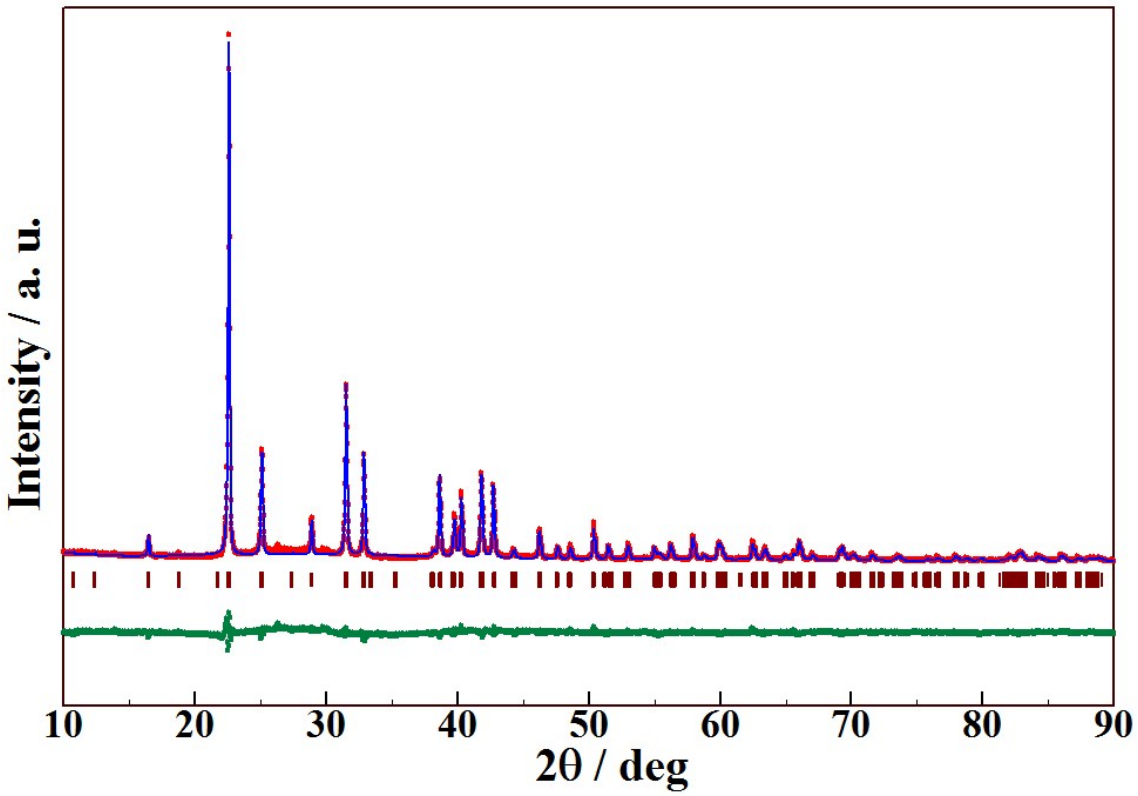

Figure S3. Observed (red + symbol), calculated (blue solid line) and difference (green solid line) patterns for the Rietveld refinement from the X-ray powder diffraction data of the synthesized σ–$(Ba_{0.72}Eu_{0.03}Mg_{0.30})_2P_2O_7$.

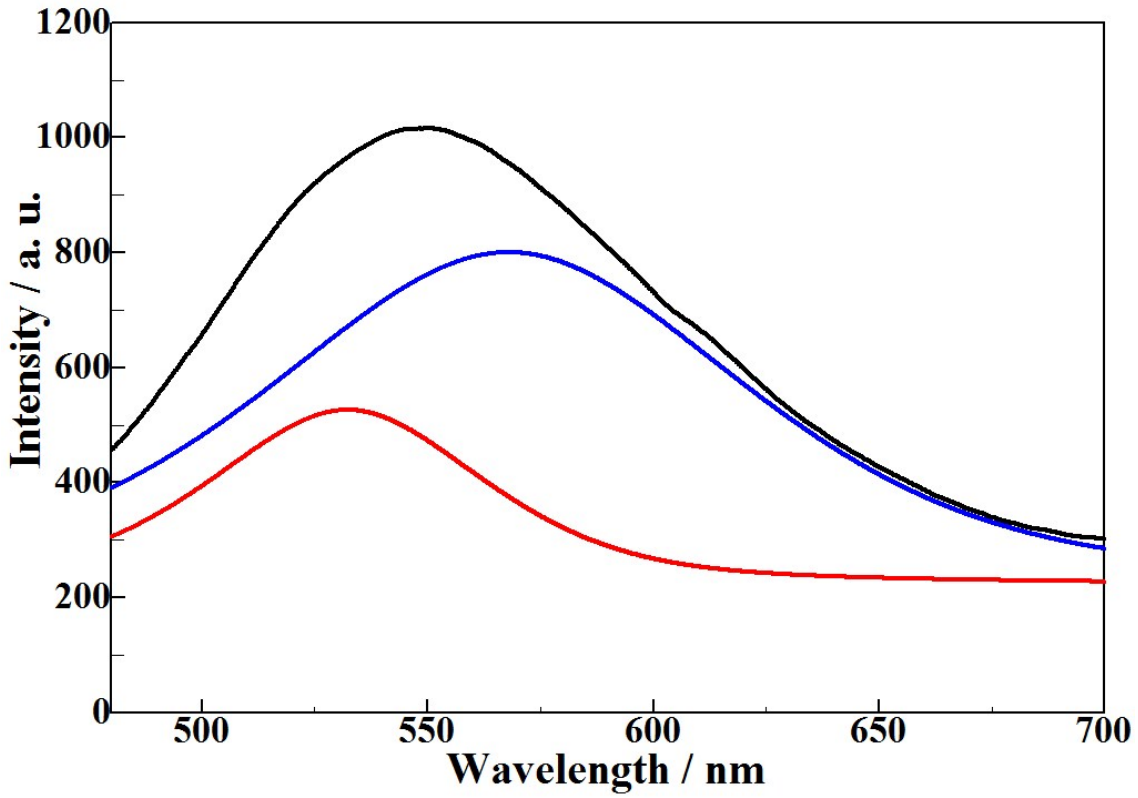

Figure S4. Observed (black line), calculated (red and blue line) patterns for the Fit Peak refinement from emission spectrum data of the synthesized σ-$(Ba_{0.72}Eu_{0.03}Mg_{0.30})_2P_2O_7$. Calculated emission spectra corresponding to BaO_9 and BaO_7 polyhedral sates are plotted by red or blue solid line, respectively.