Electronic Supplementary Information (ESI)

Crystal structure, luminescence properties and thermal stability of $BaY_{2-x}Eu_xGe_3O_{10}$ phosphors with high colour purity for blue-excited pc-LEDs

Olga A. Lipina[a]*, Ludmila L. Surat[a], Yana V. Baklanova[a], Leonid Yu. Mironov[b], Andrey N. Enyashin[a], Alexander Yu. Chufarov[a], Alexander P. Tyutyunnik[a], Vladimir G. Zubkov[a]

[a]*Institute of Solid State Chemistry, UB RAS, 620990 Ekaterinburg, Russia*

[b]*ITMO University, 197101, St. Petersburg, Russia*

* Corresponding author. E-Mail: LipinaOlgaA@yandex.ru

a) *b*)

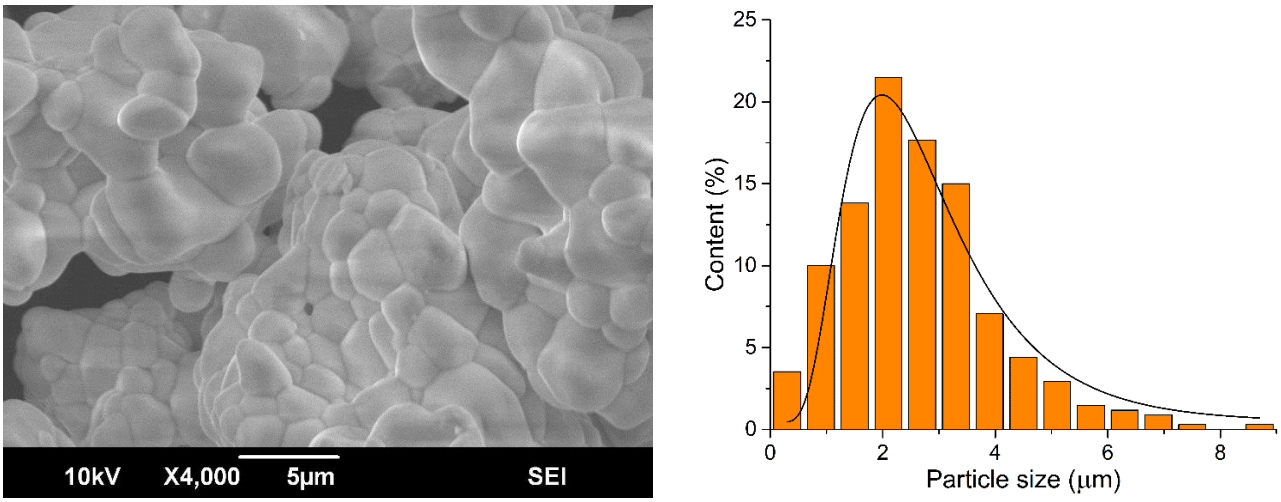

Fig. S1 SEM image of $BaY_{1.4}Eu_{0.6}Ge_3O_{10}$ powder (a) and the particle size distribution histogram with log-normal distribution fit (b).

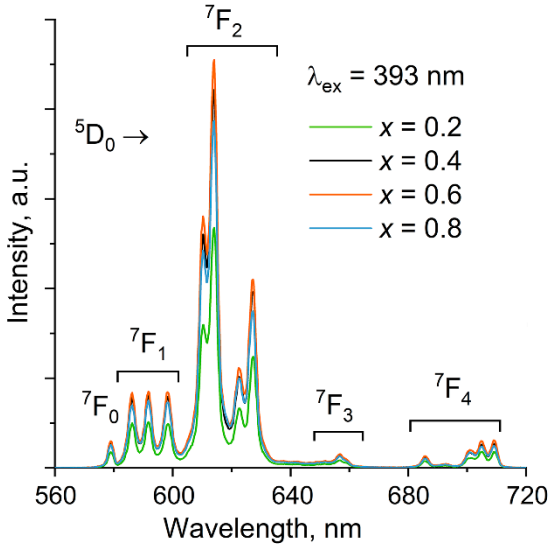

Fig. S2 The PL spectra of $BaY_{2-x}Eu_xGe_3O_{10}$ (x = 0.2, 0.4, 0.6 and 0.8) measured under 393 nm excitation.

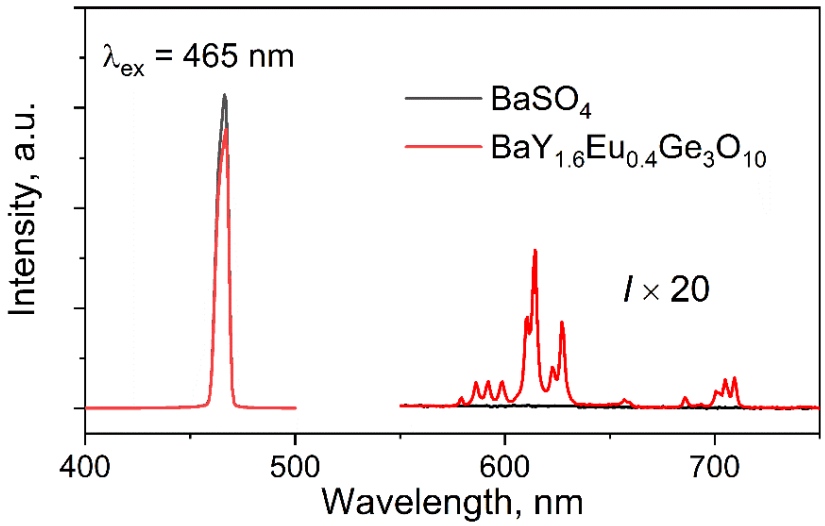

Fig. S3 The results of the measurement of the external quantum efficiency for $BaY_{1.6}Eu_{0.4}Ge_3O_{10}$ phosphor (λ_{ex} = 465 nm).

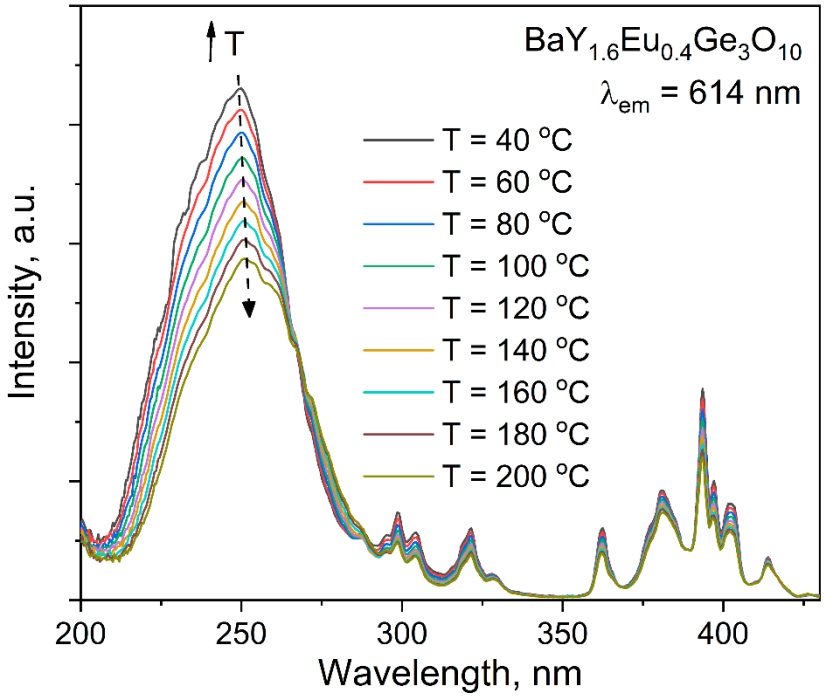

Fig. S4 The PLE spectra of $BaY_{1.6}Eu_{0.4}Ge_3O_{10}$ measured in the temperature range from 40 °C to 200 °C (λ_{em} = 614 nm).

Table S1 Atomic coordinates and thermal parameters (Å^2) for $BaY_{2-x}Eu_xGe_3O_{10}$ (x = 0.1−0.8)

Atom			x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8
Ba	2*e*	*x/a*	0.76580(32)	0.76546(31)	0.76543(25)	0.76600(32)	0.76526(31)	0.7649(4)	0.7641(4)	0.7628(5)
		y/b	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25
		z/c	0.01254(26)	0.01308(25)	0.01311(20)	0.01377(26)	0.01229(25)	0.01276(28)	0.01290(34)	0.0114(4)
		U_i/U_e*100	2.62(6)	2.50(6)	2.71(4)	2.55(8)	3.36(6)	3.42(7)	3.17(8)	5.14(11)
Y/Eu	4*f*	*x/a*	0.1542(4)	0.1540(4)	0.15315(28)	0.1541(4)	0.15444(34)	0.1549(4)	0.1544(5)	0.1557(6)
		y/b	0.10076(13)	0.10047(12)	0.10074(9)	0.10048(12)	0.10012(12)	0.10052(12)	0.10021(15)	0.10106(17)
		z/c	0.67613(25)	0.67672(24)	0.67610(19)	0.67622(26)	0.67694(23)	0.67645(27)	0.67687(31)	0.6762(4)
		U_i/U_e*100	2.45(5)	2.44(5)	2.52(4)	2.60(8)	2.83(5)	3.40(5)	3.09(6)	5.13(8)
		Fractions	0.95/0.05	0.90/0.10	0.85/0.15	0.80/0.20	0.75/0.25	0.70/0.30	0.65/0.35	0.60/0.40
Ge(1)	2*e*	*x/a*	0.5800(6)	0.5808(6)	0.58270(47)	0.5819(6)	0.5840(6)	0.5853(7)	0.5863(8)	0.5886(10)
		y/b	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25
		z/c	0.47717(46)	0.47672(44)	0.47710(35)	0.47739(46)	0.47747(44)	0.47736(48)	0.4785(6)	0.4780(7)
		U_i/U_e*100	2.32(8)	2.29(8)	2.39(6)	2.42(10)	2.74(9)	2.73(9)	2.34(11)	4.06(15)
Ge(2)	4*f*	*x/a*	0.3042(4)	0.3027(4)	0.30479(32)	0.3039(4)	0.3032(4)	0.3049(5)	0.3059(6)	0.3081(7)
		y/b	0.05303(16)	0.05299(15)	0.05364(12)	0.05329(16)	0.05360(16)	0.05370(17)	0.05349(21)	0.05388(25)
		z/c	0.20266(32)	0.20170(31)	0.20288(25)	0.20220(33)	0.20173(31)	0.20269(35)	0.2034(4)	0.2042(5)
		U_i/U_e*100	2.28(6)	2.26(6)	2.42(5)	2.28(9)	3.01(7)	3.08(7)	2.80(9)	4.59(11)
O(1)	2*e*	*x/a*	0.3436(26)	0.3388(25)	0.3448(20)	0.3357(27)	0.3428(26)	0.3383(28)	0.3405(35)	0.3442(39)
		y/b	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25
		z/c	0.5901(18)	0.5964(17)	0.5906(14)	0.5970(19)	0.5974(18)	0.5981(19)	0.5974(24)	0.5967(28)
		U_i/U_e*100	2.11(42)	1.66(39)	2.48(33)	2.65(45)	3.86(47)	3.34(48)	4.90(68)	4.8(7)
O(2)	2*e*	*x/a*	0.8842(29)	0.8893(26)	0.8806(21)	0.8867(27)	0.8862(27)	0.8951(30)	0.8943(32)	0.9048(40)
		y/b	0.25	0.25	0.25	0.25	0.25	0.25	0.25	0.25
		z/c	0.6358(20)	0.6414(18)	0.6378(15)	0.6376(18)	0.6379(18)	0.6425(20)	0.6393(21)	0.6349(27)
		U_i/U_e*100	1.86(45)	0.90(40)	1.77(35)	0.57(41)	1.81(44)	1.48(45)	1.33(46)	1.0(6)
O(3)	4*f*	*x/a*	0.5683(17)	0.5680(17)	0.5673(13)	0.5642(18)	0.5654(16)	0.5654(18)	0.5632(20)	0.5659(23)
		y/b	0.1392(7)	0.1385(7)	0.1392(5)	0.1399(7)	0.1384(7)	0.1391(7)	0.1381(8)	0.1423(8)
		z/c	0.3178(15)	0.3180(14)	0.3173(11)	0.3175(15)	0.3182(14)	0.3195(15)	0.3216(17)	0.3194(19)
		U_i/U_e*100	2.46(30)	2.42(29)	2.43(23)	2.98(33)	2.73(29)	2.22(30)	1.43(34)	1.2(4)
O(4)	4*f*	*x/a*	0.4501(18)	0.4484(18)	0.4477(14)	0.4430(19)	0.4382(17)	0.4255(19)	0.4234(23)	0.4126(28)
		y/b	-0.0692(7)	-0.0696(7)	-0.0681(6)	-0.0678(7)	-0.0688(7)	-0.0653(7)	-0.0647(9)	-0.0652(10)
		z/c	0.1777(14)	0.1777(15)	0.1779(11)	0.1821(15)	0.1827(14)	0.1791(16)	0.1818(19)	0.1757(23)
		U_i/U_e*100	1.98(31)	2.43(33)	2.62(26)	2.10(34)	2.71(34)	3.28(39)	2.94(48)	4.6(6)
O(5)	4*f*	*x/a*	0.1298(18)	0.1314(17)	0.1296(14)	0.1290(18)	0.1354(18)	0.1266(20)	0.1217(24)	0.1131(27)
		y/b	0.1182(8)	0.1194(8)	0.1209(6)	0.1192(8)	0.1212(8)	0.1259(9)	0.1285(10)	0.1309(11)
		z/c	-0.0138(15)	-0.0139(14)	-0.0151(11)	-0.0094(14)	-0.0128(15)	-0.0089(16)	-0.0062(19)	-0.0063(22)
		U_i/U_e*100	2.42(29)	2.26(28)	3.05(24)	2.01(30)	3.99(32)	3.92(34)	3.70(41)	4.3(4)
O(6)	4*f*	*x/a*	0.1021(21)	0.1136(20)	0.1142(15)	0.1085(21)	0.1103(18)	0.1065(22)	0.1010(26)	0.0875(34)
		y/b	0.0415(8)	0.0424(7)	0.0408(6)	0.0418(7)	0.0427(7)	0.0417(7)	0.0441(9)	0.0440(11)
		z/c	0.3586(15)	0.3601(14)	0.3600(11)	0.3581(15)	0.3659(13)	0.3567(16)	0.3540(19)	0.3522(24)
		U_i/U_e*100	2.71(32)	2.36(30)	2.27(23)	2.57(32)	1.97(28)	3.48(35)	3.01(41)	5.6(5)

Table S2 Selected interatomic distances (Å) for $BaY_{2-x}Eu_xGe_3O_{10}$ (x = 0.1−0.8)

	x = 0.1	x = 0.2	x = 0.3	x = 0.4	x = 0.5	x = 0.6	x = 0.7	x = 0.8
Ba-O(1)	3.223(13)	3.209(12)	3.222(10)	3.222(13)	3.196(12)	3.206(13)	3.205(17)	3.190(19)
Ba-O(2)	2.889(14)	2.872(13)	2.873(11)	2.895(13)	2.886(13)	2.884(14)	2.908(15)	2.962(18)
Ba-O(3) ×2	2.996(10)	2.999(9)	2.993(7)	2.999(10)	3.015(9)	3.016(9)	3.038(11)	3.000(12)
Ba-O(4) ×2	2.709(9)	2.704(9)	2.719(7)	2.729(9)	2.708(9)	2.717(9)	2.728(11)	2.686(13)
Ba-O(5) ×2	2.654(10)	2.657(9)	2.640(8)	2.638(10)	2.660(10)	2.581(10)	2.539(12)	2.487(14)
d_{av}**(Ba-O)**	2.854	2.850	2.850	2.856	2.856	2.840	2.840	2.812
D	0.060	0.060	0.060	0.060	0.060	0.067	0.073	0.080
Y/Eu-O(1)	2.292(9)	2.267(8)	2.299(7)	2.255(9)	2.280(8)	2.259(9)	2.273(11)	2.272(12)
Y/Eu-O(2)	2.353(9)	2.340(8)	2.363(7)	2.348(9)	2.355(9)	2.326(9)	2.329(10)	2.290(12)
Y/Eu-O(4)	2.196(10)	2.204(10)	2.216(8)	2.231(10)	2.251(9)	2.326(10)	2.338(12)	2.395(15)
Y/Eu-O(5)	2.220(10)	2.215(9)	2.215(8)	2.255(9)	2.221(10)	2.276(10)	2.307(12)	2.335(14)
Y/Eu-O(6)	2.278(10)	2.279(10)	2.285(8)	2.288(10)	2.240(9)	2.299(11)	2.307(13)	2.309(16)
Y/Eu-O(6)	2.240(10)	2.285(9)	2.272(7)	2.264(9)	2.273(8)	2.261(10)	2.263(11)	2.231(14)
d_{av}**(Y/Eu-O)**	2.263	2.265	2.275	2.274	2.270	2.291	2.303	2.305
D	0.016	0.015	0.016	0.014	0.015	0.011	0.009	0.015
Ge(1)-O(1)	1.719(15)	1.779(14)	1.730(11)	1.800(15)	1.778(15)	1.811(15)	1.798(20)	1.790(21)
Ge(1)-O(2)	1.750(14)	1.786(13)	1.730(11)	1.759(14)	1.751(14)	1.797(15)	1.779(16)	1.808(21)
Ge(1)-O(3) ×2	1.757(9)	1.761(9)	1.757(7)	1.749(9)	1.761(9)	1.748(9)	1.752(11)	1.720(11)
d_{av}**(Ge1-O)**	1.746	1.772	1.744	1.764	1.763	1.776	1.770	1.760
Ge(2)-O(3)	1.817(10)	1.819(10)	1.806(7)	1.807(10)	1.805(9)	1.803(10)	1.789(12)	1.814(13)
Ge(2)-O(4)	1.752(9)	1.753(9)	1.739(7)	1.714(9)	1.716(8)	1.649(9)	1.630(11)	1.620(13)
Ge(2)-O(5)	1.751(10)	1.750(10)	1.773(8)	1.734(10)	1.748(10)	1.781(11)	1.802(13)	1.841(15)
Ge(2)-O(6)	1.781(11)	1.737(10)	1.739(8)	1.753(10)	1.788(9)	1.758(11)	1.767(13)	1.827(15)
d_{av}**(Ge2-O)**	1.775	1.765	1.764	1.752	1.764	1.748	1.747	1.776