

Table S1. Atomic coordinates, equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) and structural occupation factor for  $x = 0.03$ .

Site	Wyckoff	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ.
Ba1	8g	0.5	0	0.13355(13)	0.0402(5)	1
M1(Sr1/Eu1)	8h	0.32846(16)	0.17154(16)	0	0.0341(8)	0.97/0.03
M2(Ba2/Sr2)	32m	0.20029(9)	-0.07166(10)	0.13446(8)	0.0361(4)	0.5/0.5
O1	16k	0.3504(10)	-0.0244(11)	0	0.030(5)	1
O2	26l	0.3724(8)	-0.1278(8)	0.2125(11)	0.040(4)	1
O3	32m	0.3840(10)	-0.2435(12)	0.3354(9)	0.065 (5)	1
O4	8h	0.1977(10)	0.3023(10)	0	0.032(6)	1
O5	32m	-0.041(3)	-0.0944(19)	0.267(4)	0.112(18)*	0.375
O6	16k	0.044(3)	-0.0964(18)	0	0.13(2)	0.75
B1	16l	0.3406(13)	-0.1594(13)	0.2963(15)	0.039(8)	1
B2	8h	0.372(2)	-0.128(2)	0	0.039(10)*	1
B3	4a	0	0	0.25	0.046(16)	1
B4	4c	0	0	0	0.028(11)*	1

Table S2. Anisotropic atomic displacement parameters ( $\text{\AA}^2$ ) for  $x = 0.03$ .

Site	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ba1	0.0446(8)	0.0446(8)	0.0313(11)	-0.0012 (10)	0	0
M1(Sr1/Eu1)	0.0414(13)	0.0414(13)	0.0196(15)	0.0276(15)	0	0
M2(Ba2/Sr2)	0.0411(8)	0.0362(7)	0.0310(7)	-0.0053(5)	0.0013(5)	0.0005(5)
O1	0.022 (8)	0.041 (9)	0.027 (8)	-0.003 (7)	0	0
O2	0.038 (6)	0.038 (6)	0.046 (10)	-0.007 (8)	0.011 (5)	0.011 (5)
O3	0.043 (7)	0.091 (10)	0.062 (9)	0.022 (8)	0.015 (6)	0.048 (8)
O4	0.036 (8)	0.036 (8)	0.024 (12)	0.024 (10)	0	0
O6	0.17 (4)	0.10 (3)	0.10 (3)	-0.02 (3)	0	0
B1	0.032 (10)	0.032 (10)	0.053 (19)	-0.014 (13)	0.001 (9)	0.001 (9)
B4	0.05 (2)	0.05 (2)	0.04 (3)	0	0	0

Table S3. Atomic coordinates, equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) and structural occupation factor for  $x = 0.06$ .

Site	Wyckoff	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ.
Ba1	8g	0.5	0	0.13349 (9)	0.0430 (4)	1
M1(Sr1/Eu1)	8h	0.3283 (1)	0.17167 (12)	0	0.0389 (6)	0.94/0.06
M2(Ba2/Sr2)	32m	0.20046 (7)	-0.07172 (7)	0.13426 (6)	0.0371 (3)	0.5/0.5
O1	16k	0.3477 (7)	-0.0240 (7)	0	0.033 (4)	1
O2	26l	0.3735 (7)	-0.1265 (7)	0.2115 (8)	0.048 (3)	1
O3	32m	0.3853 (7)	-0.2411 (9)	0.3373 (7)	0.066 (4)	1
O4	8h	0.1978 (8)	0.3022 (8)	0	0.037 (4)	1
O5	32m	-0.045 (2)	-0.0966 (16)	0.261 (3)	0.111 (12)*	0.375
O6	16k	0.0536 (19)	-0.0960 (15)	0	0.098 (11)	0.75
B1	16l	0.3398 (11)	-0.1602 (11)	0.2945 (16)	0.046 (6)	1
B2	8h	0.3765 (15)	-0.1235 (15)	0	0.031 (6)*	1

B3	4a	0	0	0.25	0.12 (6)	1
B4	4c	0	0	0	0.10 (2)	1

Table S4. Anisotropic atomic displacement parameters ( $\text{\AA}^2$ ) for  $x = 0.06$ .

Site	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ba1	0.0445 (6)	0.0445 (6)	0.0400 (8)	−0.0040 (7)	0	0
<i>M1</i> (Sr1/Eu1)	0.0448 (9)	0.0448 (9)	0.0271 (11)	0.0249 (11)	0	0
<i>M2</i> (Ba2/Sr2)	0.0392 (6)	0.0358 (5)	0.0363 (5)	−0.0044 (4)	0.0015 (4)	0.0004 (4)
O1	0.028 (6)	0.026 (6)	0.045 (6)	0.001 (5)	0	0
O2	0.060 (5)	0.060 (5)	0.026 (6)	0.003 (7)	0.007 (4)	0.007 (4)
O3	0.051 (6)	0.083 (7)	0.064 (6)	0.014 (5)	−0.004 (5)	0.023 (6)
O4	0.038 (6)	0.038 (6)	0.036 (9)	0.010 (7)	0	0
O6	0.11 (2)	0.10 (2)	0.078 (15)	0.016 (15)	0	0
B1	0.040 (7)	0.040 (7)	0.059 (14)	−0.005(10)	−0.015(8)	−0.015(8)
B3	0.010 (16)	0.010 (16)	0.18 (17)	0	0	0
B4	0.10 (3)	0.10 (3)	0.09 (5)	0	0	0

Table S5. Atomic coordinates, equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) and structural occupation factor for  $x = 0.15$ .

Site	Wyckoff	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ.
Ba1	8g	0.5	0	0.13351 (9)	0.0411 (4)	1
<i>M1</i> (Sr1/Eu1)	8h	0.32919 (11)	0.1708 (1)	0	0.0335 (5)	0.85/0.15
<i>M2</i> (Ba2/Sr2)	32m	0.20070 (7)	−0.07170 (7)	0.13414 (5)	0.0303 (3)	0.5/0.5
O1	16k	0.3482 (8)	−0.0249 (8)	0	0.029 (3)	1
O2	26l	0.3718 (7)	−0.1282 (7)	0.2113 (7)	0.041 (3)	1
O3	32m	0.3842 (8)	−0.2430 (9)	0.3390 (7)	0.062 (4)	1
O4	8h	0.1971 (8)	0.3029 (8)	0	0.032 (4)	1
O5	32m	−0.095 (2)	−0.042 (3)	0.226 (3)	0.124 (15)*	0.375
O6	16k	0.050 (2)	−0.0960 (17)	0	0.120 (14)	0.75
B1	16l	0.3404 (9)	−0.1596 (9)	0.2955 (10)	0.026 (4)	1
B2	8h	0.3752 (14)	−0.1248 (14)	0	0.024 (5)*	1
B3	4a	0	0	0.25	0.064 (14)*	1
B4	4c	0	0	0	0.11 (3)	1

Table S6. Anisotropic atomic displacement parameters ( $\text{\AA}^2$ ) for  $x = 0.15$ .

Site	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ba1	0.0431 (6)	0.0431 (6)	0.0371 (8)	−0.0027 (7)	0	0
<i>M1</i> (Sr1/Eu1)	0.0415 (9)	0.0415 (9)	0.0175 (9)	0.0218 (11)	0	0
<i>M2</i> (Ba2/Sr2)	0.0357 (6)	0.0298 (6)	0.0253 (5)	−0.0042 (4)	0.0017 (3)	−0.0002 (3)
O1	0.025 (6)	0.033 (6)	0.028 (5)	−0.005 (5)	0	0
O2	0.050 (5)	0.050 (5)	0.023 (5)	−0.001 (6)	0.014 (4)	0.014 (4)
O3	0.046 (6)	0.083 (8)	0.057 (6)	0.007 (6)	−0.001 (5)	0.016 (6)

O4	0.030 (6)	0.030 (6)	0.038 (9)	0.003 (7)	0	0
O6	0.11 (2)	0.08 (2)	0.17 (3)	0.021 (18)	0	0
B1	0.031 (6)	0.031 (6)	0.018 (7)	−0.006 (8)	−0.008 (5)	−0.008 (5)
B4	0.09 (4)	0.09 (4)	0.17 (8)	0	0	0

Table S7. Atomic coordinates, equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) and structural occupation factor for  $x = 0.20$ .

Site	Wyckoff	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ.
Ba1	8g	0.5	0	0.13417 (15)	0.0597 (7)	1
M1(Sr1/Eu1)	8h	0.32951 (16)	0.17049 (16)	0	0.0400 (8)	0.8/0.2
M2(Ba2/Sr2)	32m	0.20116 (9)	−0.07164 (9)	0.13381 (7)	0.0362 (4)	0.5/0.5
O1	16k	0.3487 (11)	−0.0252 (11)	0	0.036 (5)	1
O2	26l	0.3710 (9)	−0.1290 (9)	0.2142 (11)	0.052 (5)	1
O3	32m	0.3856 (10)	−0.2418 (12)	0.3378 (10)	0.069 (5)	1
O4	8h	0.1960 (12)	0.3040 (12)	0	0.048 (7)	1
O5	32m	−0.092 (3)	−0.041 (4)	0.221 (4)	0.15 (3)*	0.375
O6	16k	0.048 (3)	−0.095 (2)	0	0.15 (2)	0.75
B1	16l	0.3407 (15)	−0.1593 (15)	0.2937 (19)	0.043 (7)	1
B2	8h	0.3784 (19)	−0.1216 (19)	0	0.027 (7)*	1
B3	4a	0	0	0.25	0.059(17)*	1
B4	4c	0	0	0	0.047(17)	1

Table S8. Anisotropic atomic displacement parameters ( $\text{\AA}^2$ ) for  $x = 0.20$ .

Site	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ba1	0.0526 (10)	0.0526 (10)	0.0738 (15)	−0.0039 (12)	0	0
M1(Sr1/Eu1)	0.0453 (13)	0.0453 (13)	0.0292 (14)	0.0214 (16)	0	0
M2(Ba2/Sr2)	0.0400 (8)	0.0327 (7)	0.0358 (7)	−0.0053 (5)	0.0026 (5)	−0.0004 (5)
O1	0.028 (9)	0.039 (9)	0.041 (8)	−0.004 (7)	0	0
O2	0.054 (7)	0.054 (7)	0.047 (10)	−0.003 (9)	0.017 (6)	0.017 (6)
O3	0.047 (8)	0.077 (10)	0.083 (9)	0.026 (8)	0.004 (7)	0.036 (8)
O4	0.049 (10)	0.049 (10)	0.047 (14)	0.015 (12)	0	0
O6	0.11 (4)	0.13 (4)	0.22 (4)	0.01 (3)	0	0
B1	0.044 (11)	0.044 (11)	0.040 (16)	−0.012 (15)	−0.018 (9)	−0.018 (9)
B4	0.023 (19)	0.023 (19)	0.09 (4)	0	0	0

Table S9. Atomic coordinates, equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) and structural occupation factor for  $x = 0.25$ .

Site	Wyckoff	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ.
Ba1	8g	0.5	0	0.1341 (2)	0.0630 (10)	1
M1(Sr1/Eu1)	8h	0.3305 (2)	0.1695 (2)	0	0.0442 (11)	0.75/0.25

<i>M2</i> (Ba2/Sr2/ Eu2)	<i>32m</i>	0.20055 (13)	−0.07142 (13)	0.13402 (11)	0.0431 (6)	0.5/0.48/ 0.02
O1	<i>16k</i>	0.3473 (16)	−0.0233 (12)	0	0.043 (6)	1
O2	<i>26l</i>	0.3708 (10)	−0.1292 (10)	0.2134 (14)	0.043 (6)	1
O3	<i>32m</i>	0.3820 (12)	−0.2440 (12)	0.3367 (11)	0.055 (6)	1
O4	<i>8h</i>	0.3047 (14)	−0.1953 (14)	0	0.049 (9)	1
O5	<i>19j</i>	−0.1068 (15)	0.00 (2)	0.25 (10)	0.20 (9)*	0.75
O6	<i>16k</i>	0.027 (6)	−0.112 (3)	0	0.17 (3)	0.75
B1	<i>16l</i>	0.335 (2)	−0.165 (2)	0.295 (2)	0.070 (13)*	1
B2	<i>8h</i>	0.3780 (14)	−0.1220 (14)	0	0.009 (7)*	1
B3	<i>4a</i>	0	0	0.25	0.045 (1)	1
B4	<i>4c</i>	0	0	0	0.07 (3)*	1

Table S10. Anisotropic atomic displacement parameters ( $\text{\AA}^2$ ) for  $x = 0.25$ .

Site	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ba1	0.0551 (13)	0.0551 (13)	0.079 (2)	−0.0024(16)	0	0
<i>M1</i> (Sr1/Eu1)	0.0500 (18)	0.0500 (18)	0.033 (2)	0.020 (2)	0	0
<i>M2</i> (Ba2/Sr2/ Eu2)	0.0467 (12)	0.0395 (11)	0.0430 (9)	−0.0074 (8)	0.0040 (8)	−0.0021 (8)
O1	0.058 (12)	0.022 (9)	0.050 (9)	−0.015 (8)	0	0
O2	0.058 (12)	0.022 (9)	0.050 (9)	−0.015 (8)	0	0
O3	0.055 (11)	0.037 (9)	0.072 (12)	0.030 (8)	−0.029 (8)	0.007 (8)
O4	0.071 (14)	0.071 (14)	0.006 (13)	0.003 (18)	0	0
O6	0.28 (7)	0.03 (3)	0.19(5)	0.02 (3)	0	0
B3	0.0240 (5)	0.0240 (5)	0.086 (3)	0	0	0

Table S11. Refined number of electrons per site and assignment for cation sites in the structure of  $\text{Ba}_3(\text{Sr}_{3-1.5x}\text{Eu}_x)\text{B}_4\text{O}_{12}$  phosphors.

Site (new)	SC	SOF	SSF <sub>exp</sub> [ $e^-$ ]	Assigned occupancy	SSF <sub>calc</sub> [ $e^-$ ]
$x = 0.03$					
Ba1	Sr	1.43	54.27	Ba <sub>1.00</sub>	56
Sr1	Sr	1.017	38.65	Sr <sub>0.945</sub> Eu <sub>0.03</sub>	38.18
Sr/Ba1	Sr	1.24	47.12	Sr <sub>0.50</sub> Ba <sub>0.50</sub>	47.00
$x = 0.06$					
Ba1		1.42	54.05	Ba <sub>1.00</sub>	56
Sr1		1.03	39.09	Sr <sub>0.91</sub> Eu <sub>0.06</sub>	38.36
Sr/Ba1		1.26	47.82	Sr <sub>0.50</sub> Ba <sub>0.50</sub>	47.00
$x = 0.15$					
Ba1	Sr	1.41	53.64	Ba <sub>1.00</sub>	56
Sr1	Sr	1.06	40.18	Sr <sub>0.775</sub> Eu <sub>0.15</sub>	38.90
Sr/Ba1	Sr	1.280	48.58	Sr <sub>0.50</sub> Ba <sub>0.50</sub>	47.00
$x = 0.20$					
Ba1	Sr	1.38	52.41	Ba <sub>1.00</sub>	56
Sr1	Sr	1.09	41.39	Sr <sub>0.70</sub> Eu <sub>0.20</sub>	39.2
Sr/Ba1	Sr	1.29	49.12	Sr <sub>0.50</sub> Ba <sub>0.50</sub>	47.00

$x = 0.25$					
Ba1	Sr	1.01	56.34	Ba <sub>1.00</sub>	56
Sr1	Sr	1.09	41.43	Sr <sub>0.70</sub> Eu <sub>0.20</sub>	39.2
Sr/Ba1	Sr	1.30	49.21	Sr <sub>0.48125</sub> Ba <sub>0.50</sub> Eu <sub>0.125</sub>	47.075

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\*SC = scattering curve used to refine site occupancy; SOF = refined site-occupation factor; SSF<sub>exp</sub> and SSF<sub>calc</sub> = experimental and calculated electrons per site