Electronic Supplementary Material (ESI) for RSC Advances.

Site occupancy and photoluminescence properties of Eu^{3+}-activated $Ba_2ZnB_2O_6$ phosphor

Huan Yi[a], Fang Li[a], Li Wu[a,*], Liwei Wu[a], Hongrun Wang[b], Biao Wang[b], Yi Zhang[b,*], Yongfa Kong[a], and Jingjun Xu[a]

a The MOE key laboratory of weak-Light Nonlinear Photonics, School of Physics, Nankai University, Tianjin 300071. Email: lwu@nankai.edu.cn; Tel: +86-22-23506257, Fax: +86-22-23505409

b Institute of Photo-electronic Thin Film Devices and Technology and Tianjin Key Laboratory of Photo-electronic Thin Film Devices and Technology, Nankai University, Tianjin 300071, China. Email: yizhang@nankai.edu.cn, Tel: +86-22-23508572-8018, Fax: +86-22-23508912

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å) for $Ba_2ZnB_2O_6$:0.05Eu^{3+} together with the occupancy.

Atom	Site	x	y	z	Occupancy
Ba1	4 a	0.3836(4)	0.6723(3)	0.3789(4)	1.0
Ba2	4 a	0.3857(2)	0.2058(3)	0.1685(3)	1.0
Ba3	4 a	0.1134(4)	0.1312(2)	0.1152(4)	1.0
Ba4	4 a	0.0984(3)	0.6874(4)	0.4074(2)	1.0
Zn1	4 a	0.2313(3)	0.0108(4)	0.4013(4)	0.975(3)
Eu1	4 a	0.2313(3)	0.0108(4)	0.4013(4)	0.025(3)
Zn2	4 a	0.2097(4)	0.5061(4)	0.1320 (3)	0.972(3)
Eu2	4 a	0.2097 (4)	0.5061(4)	0.1320(3)	0.028(3)
B1	4 a	0.0179(3)	0.4369(5)	0.1695(2)	1.0
B2	4 a	0.2400(4)	0.8793(2)	0.1520(7)	1.0
B3	4 a	0.2277(3)	0.3588(4)	0.4223(5)	1.0
B4	4 a	0.0082(3)	0.0436(4)	0.4125(3)	1.0
O1	4 a	0.4683(4)	0.6893(5)	0.1619(3)	1.0
O2	4 a	0.4792(3)	0.4630(5)	0.2613(3)	1.0
O3	4 a	0.0902(2)	0.4674(4)	0.0990(3)	1.0
O4	4 a	0.2508(3)	0.8505(5)	0.0189(5)	1.0
O5	4 a	0.2386(4)	0.7233(3)	0.2312(4)	1.0
O6	4 a	0.2751(2)	0.9702(2)	0.2312(3)	1.0
O7	4 a	0.2181(3)	0.4733(4)	0.4982(3)	1.0
O8	4 a	0.2400(3)	0.3177(4)	0.3007(3)	1.0
O9	4 a	0.2510(4)	0.2347(4)	0.4874(3)	1.0
O10	4 a	0.0207(3)	0.8684(3)	0.0058(3)	1.0
O11	4 a	0.4607(3)	0.0924(3)	0.3809(5)	1.0
O12	4 a	0.0930(3)	0.0049(4)	0.3933(4)	1.0