

Electronic Supplementary Information

Eu²⁺ doped NaBa₄(AlB₄O₉)₂X₃ (X = Cl, Br) phosphors with intense two-center blue-emission and high color purity for n-UV pumped white-light-emitting diodes

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Table S1. A comparison of some recently reported blue-emitting phosphors with high color purity.

Materials	Synthesis Temp. (°C)	Color coordinate	Excitation band (nm)	PL FWHM (nm)	Efficiency or Intensity	Color purity
SrB ₂ O ₄ :Eu ²⁺ [1]	800	(0.1480, 0.0400)	270-350	~ 45	Not reported	97.0%
NaSrBO ₃ :Ce ³⁺ [2]	850	(0.1583, 0.0493)	325-390	~ 67	External QE 89% of that for BAM:Eu ²⁺	Not indexed
K ₂ Al ₂ B ₂ O ₇ :Eu ²⁺ [3]	1000	(0.147, 0.051)	230-420	~ 50	Integrated PL intensity ~58% of that for BAM:Eu ²⁺	Not indexed
Sr ₅ (PO ₄) ₃ Cl:Eu ²⁺ [4]	1050	(0.1540, 0.0230)	240-420	~ 32	Internal QE 90% of that for BAM:Eu ²⁺	99.0%
NBAC: Eu ²⁺ (this work)	850	(0.1578, 0.0248)	240-420	37	Integrated PL intensity 114% of that for BAM:Eu ²⁺	98.65%
NBAB: Eu ²⁺ (this work)	850	(0.1584, 0.0196)	250-420	33	Integrated PL intensity 129% of that for BAM:Eu ²⁺	99.58%

Table S2. The refined positions of all atoms for NBAC: 0.1Eu²⁺ (a) and NBAB: 0.1Eu²⁺ (b) phosphors.

Sample		NaBa _{3.9} Eu _{0.1} (AlB ₄ O ₉) ₂ Cl ₃				
Atom	Wyckoff site	x	y	z	Occupancy	Uiso
Na(1)	8d	0.000	0.000	-0.128	0.980	0.079
Eu(1)	8d	0.000	0.000	-0.128	0.020	0.079
Ba	8d	0.983	0.727	0.224	0.975	0.023
Eu(2)	2a	0.983	0.727	0.224	0.020	0.023
Na(2)	2a	0.983	0.727	0.224	0.005	0.023
Al	4c	0.297	0.703	0.218	1.000	0.017
B(1)	4c	0.234	0.767	0.583	1.000	0.017
B(2)	4c	0.185	0.815	-0.08	1.000	0.010
B(3)	8d	0.533	0.733	0.181	1.000	0.013
O(1)	8d	0.116	0.743	0.545	1.000	0.024
O(2)	8d	0.063	0.798	0.869	1.000	0.018
O(3)	4c	0.303	0.697	0.471	1.000	0.011
O(4)	4c	0.200	0.800	0.124	1.000	0.015
O(5)	4c	0.255	0.745	-0.204	1.000	0.014
O(6)	8d	0.428	0.740	0.125	1.000	0.028
Cl(1)	2a	0.000	0.000	0.282	1.000	0.012
Cl(2)	4b	0.000	0.500	0.440	1.000	0.084
Sample		NaBa _{3.9} Eu _{0.1} (AlB ₄ O ₉) ₂ Br ₃				
Atom	Wyckoff site	x	y	z	Occupancy	Uiso
Na(1)	2a	0.500	0.500	0.865	0.980	0.174
Eu(1)	2a	0.500	0.500	0.865	0.020	0.174
Ba	8d	0.517	0.766	0.487	0.975	0.027
Eu(2)	8d	0.517	0.766	0.487	0.020	0.027
Na(2)	8d	0.517	0.766	0.487	0.005	0.023
Al	4c	0.197	0.803	0.471	1.000	0.016
B(1)	8d	0.465	0.734	1.029	1.000	0.013
B(2)	4c	0.314	0.686	0.791	1.000	0.008
B(3)	4c	0.268	0.732	0.134	1.000	0.007
O(1)	4c	0.198	0.802	0.243	1.000	0.007
O(2)	8d	0.072	0.764	0.587	1.000	0.014
O(3)	4c	0.297	0.703	0.588	1.000	0.010
O(4)	8d	0.435	0.705	0.841	1.000	0.012
O(5)	4c	0.246	0.754	0.915	1.000	0.004
O(6)	8d	0.386	0.756	0.166	1.000	0.015
Br(1)	2a	0.500	0.500	0.406	1.000	0.045
Br(2)	4b	0.500	1.000	0.273	1.000	0.139

Reference

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