Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Sm^{3+} and Eu^{3+} codoped $SrBi_2B_2O_7$: a red-emitting phosphor with improved thermal stability

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Table S1. Fractional Atomic Coordinates, Equivalent Isotropic Displacement Parameters (Å²) and Occupancy for Sr(Bi, M)$_2$B$_2$O$_7$ (M=Sm, Eu) at room temperature

	site	*x*	*y*	*z*	*Ueq*	occupancy
			$SrBi_{1.96}Sm_{0.04}B_2O_7$			
Sr	6c	0.9825(1)	0.3255(5)	0	0.0182(4)	1.0000
Bi1	6c	0.3095(1)	0.3323(2)	0.8385(4)	0.0197(6)	0.978(4)
Sm1	6c	0.3095(1)	0.3323(2)	0.8385(4)	0.0197(6)	0.021(4)
Bi2	6c	0.3290(2)	0.3533(2)	0.1625(8)	0.0232(3)	0.983(8)
Sm2	6c	0.3290(2)	0.3533(2)	0.1625(8)	0.0232(3)	0.016(8)
B1	2a	0	0	0.1159(10)	0.0655(8)	1.0000
B2	2b	0.33333	0.66667	0.1086(7)	0.0617(8)	1.0000
B3	2b	0.66667	0.33333	0.1694(8)	0.0668(7)	1.0000
B4	2a	0	0	0.3516(5)	0.0595(4)	1.0000
B5	2b	0.33333	0.66667	0.3558(10)	0.0648(6)	1.0000
B6	2b	0.66667	0.33333	0.3639(8)	0.0670(5)	1.0000
O1	6c	-0.1620(12)	-0.1486(12)	0.1287(5)	0.0446(1)	1.0000
O2	6c	0.3302(12)	0.8261(13)	0.1235(5)	0.0451(7)	1.0000
O3	6c	0.8232(13)	0.3348(2)	0.1453(6)	0.0436(4)	1.0000
O4	6c	-0.1477(9)	0.0110(14)	0.3750(5)	0.0464(7)	1.0000
O5	6c	0.3354(10)	0.5147(11)	0.3528(6)	0.0459(6)	1.0000
O6	6c	0.5204(11)	0.3460(9)	0.3817(5)	0.0423(9)	1.0000
O7	6c	0.3761(6)	0.3431(10)	0	0.0401(7)	1.0000
			$SrBi_{1.94}Eu_{0.06}B_2O_7$			
Sr	6c	0.9839(1)	0.3279(6)	0	0.0186(5)	1.0000
Bi1	6c	0.3159(2)	0.3383(2)	0.8396(4)	0.0212(3)	0.964(5)
Eu1	6c	0.3159(2)	0.3383(2)	0.8396(4)	0.0212(3)	0.035(5)
Bi2	6c	0.3376(2)	0.3604(1)	0.1625(4)	0.0198(6)	0.979(1)
Eu2	6c	0.3376(2)	0.3604(1)	0.1625(4)	0.0198(6)	0.021(1)
B1	2a	0	0	0.1253(6)	0.0599(4)	1.0000
B2	2b	0.33333	0.66667	0.1086(3)	0.0664(7)	1.0000
B3	2b	0.66667	0.33333	0.1650(8)	0.0610(3)	1.0000
B4	2a	0	0	0.3793(10)	0.0651(5)	1.0000
B5	2b	0.33333	0.66667	0.3854(9)	0.0659(8)	1.0000
B6	2b	0.66667	0.33333	0.3637(12)	0.0587(4)	1.0000
O1	6c	-0.1659(11)	-0.1471(11)	0.1261(6)	0.0446(6)	1.0000
O2	6c	0.3326(7)	0.8187(15)	0.1282(11)	0.0438(5)	1.0000
O3	6c	0.8327(7)	0.3594(6)	0.1491(9)	0.0457(3)	1.0000
O4	6c	-0.1280(12)	0.0165(9)	0.3497(13)	0.0451(7)	1.0000
O5	6c	0.3257(12)	0.5177(9)	0.3532(8)	0.0462(4)	1.0000
O6	6c	0.5252(11)	0.3420(6)	0.3665(4)	0.0422(8)	1.0000
O7	6c	0.3759(13)	0.3381(11)	0	0.0436(3)	1.0000
			$SrBi_{1.90}Sm_{0.04}Eu_{0.06}B_2O_7$			
Sr	6c	0.9826(4)	0.3273(3)	0	0.0281(1)	1.0000
Bi1	6c	0.3169(7)	0.3380(9)	0.8425(6)	0.0219(7)	0.946(1)
Sm1	6c	0.3169(7)	0.3380(9)	0.8425(6)	0.0219(7)	0.022(1)
Eu1	6c	0.3169(7)	0.3380(9)	0.8425(6)	0.0219(7)	0.032(1)
Bi2	6c	0.3375(6)	0.3607(4)	0.1666(6)	0.0248(2)	0.962(1)
Sm2	6c	0.3375(6)	0.3607(4)	0.1666(6)	0.0248(2)	0.015(1)
Eu2	6c	0.3375(6)	0.3607(4)	0.1666(6)	0.0248(2)	0.023(1)
B1	2a	0	0	0.1220(8)	0.0639(5)	1.0000
B2	2b	0.33333	0.66667	0.0991(6)	0.0616(8)	1.0000
B3	2b	0.66667	0.33333	0.1407(12)	0.0622(6)	1.0000
B4	2a	0	0	0.3583(5)	0.0636(2)	1.0000
B5	2b	0.33333	0.66667	0.3616(10)	0.0621(4)	1.0000
B6	2b	0.66667	0.33333	0.3619(3)	0.0615(7)	1.0000
O1	6c	-0.1649(13)	-0.1552(13)	0.1221(5)	0.0459(2)	1.0000
O2	6c	0.3335(7)	0.8213(15)	0.1294(9)	0.0478(2)	1.0000
O3	6c	0.8328(10)	0.3510(13)	0.1470(8)	0.0405(7)	1.0000
O4	6c	-0.1392(13)	0.0125(12)	0.3574(8)	0.0480(6)	1.0000
O5	6c	0.3290(5)	0.5200(7)	0.3426(12)	0.0481(4)	1.0000

O6	6c	0.5270(7)	0.3457(5)	0.3722(3)	0.0419(1)	1.0000
O7	6c	0.3706(9)	0.3312(6)	0	0.0474(1)	1.0000

Table S2. Fractional Atomic Coordinates, Equivalent Isotropic Displacement Parameters (Å^2) and Occupancy for Sr(Bi, M)$_2$B$_2$O$_7$ (M=Sm, Eu) at 150^{o}C

	site	*x*	*y*	*z*	*Ueq*	occupancy
			$SrBi_{1.96}Sm_{0.04}B_2O_7$			
Sr	6c	0.9841(2)	0.3381(9)	0	0.0253(5)	1.0000
Bi1	6c	0.3097(2)	0.3331(3)	0.8399(8)	0.0204(7)	0.980(6)
Sm1	6c	0.3097(2)	0.3331(3)	0.8399(8)	0.0204(7)	0.019(6)
Bi2	6c	0.3310(3)	0.3546(2)	0.1632(8)	0.0192(4)	0.982(1)
Sm2	6c	0.3310(3)	0.3546(2)	0.1632(8)	0.0192(4)	0.018(1)
B1	2a	0	0	0.1203(9)	0.0642(5)	1.0000
B2	2b	0.33333	0.66667	0.1075(6)	0.0625(3)	1.0000
B3	2b	0.66667	0.33333	0.1403(4)	0.0668(2)	1.0000
B4	2a	0	0	0.3364(6)	0.0595(6)	1.0000
B5	2b	0.33333	0.66667	0.3760(3)	0.0647(7)	1.0000
B6	2b	0.66667	0.33333	0.3728(9)	0.0670(9)	1.0000
O1	6c	-0.1662(5)	-0.1486(8)	0.1267(5)	0.0368(5)	1.0000
O2	6c	0.3307(2)	0.8233(6)	0.1282(8)	0.0351(7)	1.0000
O3	6c	0.8305(2)	0.3566(5)	0.1589(8)	0.0346(8)	1.0000
O4	6c	-0.1343(7)	0.0147(3)	0.3535(3)	0.0371(4)	1.0000
O5	6c	0.3303(8)	0.5176(2)	0.3441(7)	0.0359(6)	1.0000
O6	6c	0.5276(2)	0.3446(6)	0.3680(5)	0.0344(1)	1.0000
O7	6c	0.3841(9)	0.3496(5)	0	0.0378(4)	1.0000
			$SrBi_{1.94}Eu_{0.06}B_2O_7$			
Sr	6c	0.9841(2)	0.3289(10)	0	0.0235(2)	1.0000
Bi1	6c	0.3145(2)	0.3382(3)	0.8395(8)	0.0168(4)	0.969(1)
Eu1	6c	0.3145(2)	0.3382(3)	0.8395(8)	0.0168(4)	0.031(1)
Bi2	6c	0.3374(3)	0.3604(2)	0.1628(8)	0.0153(7)	0.974(7)
Eu2	6c	0.3374(3)	0.3604(2)	0.1628(8)	0.0153(7)	0.025(7)
B1	2a	0	0	0.1196(11)	0.0624(3)	1.0000
B2	2b	0.33333	0.66667	0.1104(7)	0.0621(6)	1.0000
B3	2b	0.66667	0.33333	0.1586(3)	0.0618(1)	1.0000
B4	2a	0	0	0.3629(5)	0.0621(8)	1.0000
B5	2b	0.33333	0.66667	0.3684(7)	0.0635(6)	1.0000
B6	2b	0.66667	0.33333	0.3502(12)	0.0612(4)	1.0000
O1	6c	-0.1675(9)	-0.1494(11)	0.1239(6)	0.0446(5)	1.0000
O2	6c	0.3333(5)	0.8245(13)	0.1272(9)	0.0438(2)	1.0000
O3	6c	0.8378(14)	0.3633(9)	0.1503(8)	0.0399(6)	1.0000
O4	6c	-0.1387(5)	0.0142(7)	0.3568(11)	0.0412(3)	1.0000
O5	6c	0.3285(6)	0.5179(13)	0.3446(9)	0.0401(4)	1.0000
O6	6c	0.5277(12)	0.3457(11)	0.3557(9)	0.0422(5)	1.0000
O7	6c	0.3745(13)	0.3367(9)	0	0.0459(7)	1.0000
			$SrBi_{1.90}Sm_{0.04}Eu_{0.06}B_2O_7$			
Sr	6c	0.9824(1)	0.3280(5)	0	0.0213(5)	1.0000
Bi1	6c	0.3167(13)	0.3382(8)	0.8390(5)	0.0188(7)	0.951(1)
Sm1	6c	0.3167(13)	0.3382(8)	0.8390(5)	0.0188(7)	0.020(1)
Eu1	6c	0.3167(1)	0.3382(8)	0.8390(5)	0.0188(7)	0.029(1)
Bi2	6c	0.3366(2)	0.3574(1)	0.1632(5)	0.0181(4)	0.957(1)
Bi2	6c	0.3366(2)	0.3574(1)	0.1632(5)	0.0181(4)	0.017(1)
Bi2	6c	0.3366(2)	0.3574(1)	0.1632(5)	0.0181(4)	0.026(1)
B1	2a	0	0	0.1253(6)	0.0624(4)	1.0000
B2	2b	0.33333	0.66667	0.1086(13)	0.0621(6)	1.0000
B3	2b	0.66667	0.33333	0.1650(8)	0.0618(8)	1.0000
B4	2a	0	0	0.3793(6)	0.0635(4)	1.0000
B5	2b	0.33333	0.66667	0.3854(9)	0.0626(6)	1.0000
B6	2b	0.66667	0.33333	0.3637(11)	0.0631(2)	1.0000

O1	6c	-0.1659(11)	-0.1471(11)	0.1261(6)	0.0446(5)	1.0000
O2	6c	0.3326(7)	0.8187(15)	0.1282(11)	0.0438(5)	1.0000
O3	6c	0.8327(7)	0.3594(6)	0.1491(9)	0.0399(2)	1.0000
O4	6c	-0.1280(13)	0.0165(9)	0.3497(13)	0.0412(7)	1.0000
O5	6c	0.3257(3)	0.5177(9)	0.3532(8)	0.0401(5)	1.0000
O6	6c	0.5252(11)	0.3420(6)	0.3665(4)	0.0390(3)	1.0000
O7	6c	0.3813(9)	0.3491(16)	0	0.0405(7)	1.0000

Table S3. Selected average bond lengths (Å) of Bi–O in $Sr(Bi, M)_2B_2O_7$ (M=Sm, Eu)

	$SrBi_{1.96}Sm_{0.04}B_2O_7$		$SrBi_{1.94}Eu_{0.06}B_2O_7$		$SrBi_{1.90}Sm_{0.04}Eu_{0.06}B_2O_7$	
	Bi1(Sm) –O	Bi2(Sm) –O	Bi1(Eu) –O	Bi2(Eu) –O	Bi1(Sm, Eu) –O	Bi2(Sm, Eu) –O
25 °C	2.634	2.638	2.631	2.634	2.624	2.627
150 °C	2.627	2.632	2.623	2.627	2.618	2.622