Electronic Supplementary Material (ESI) for Dalton Transactions.


Table S1. The atomic coordinates, site occupancies and temperature factors of NBB: $0.03Ce^{3+}$ samples

| Atoms | x | y | z | Usio | Occupy |
|---|---|---|---|---|---|
| **Ba** | **0** | **0** | **0.0082** | **0.02491** | **1** |
| **Na** | **0** | **0** | **0.2301** | **0.01275** | **1** |
| **B1** | **0.3854** | **0.2710** | **0.0567** | **0.00257** | **1** |
| **B2** | **0.4538** | **0.3987** | **0.1787** | **0.00132** | **1** |
| **B3** | **0.2095** | **0.3127** | **0.1187** | **0.03596** | **1** |
| **O1** | **0.4797** | **0.3384** | **0.1213** | **0.03203** | **1** |
| **O2** | **0.2504** | **0.2494** | **0.0630** | **0.03903** | **1** |
| **O3** | **0.2127** | **0.4265** | **0.0715** | **0.03898** | **1** |
| **O4** | **0.3679** | **0.4212** | **0.1739** | **0.00756** | **1** |
| **O5** | **0.0954** | **0.2337** | **0.1705** | **0.00562** | **1** |

Table S2. The atomic coordinates, site occupancies and temperature factors of NBB: $0.03Ce^{3+}$, $0.03Mn^{2+}$ samples

| Atoms | x | y | z | Usio | Occupy |
|---|---|---|---|---|---|
| **Ba** | **0** | **0** | **0.0047** | **0.02067** | **1** |
| **Na** | **0** | **0** | **0.2212** | **0.01872** | **1** |
| **B1** | **0.3964** | **0.2605** | **0.0554** | **0.02870** | **1** |

| | | | | | |
|---|---|---|---|---|---|
| **B2** | **0.4363** | **0.4008** | **0.1836** | **0.03952** | **1** |
| **B3** | **0.2338** | **0.3603** | **0.1012** | **0.01612** | **1** |
| **O1** | **0.4726** | **0.3434** | **0.1179** | **0.00626** | **1** |
| **O2** | **0.2706** | **0.2492** | **0.0546** | **0.02157** | **1** |
| **O3** | **0.2067** | **0.4305** | **0.0643** | **0.01706** | **1** |
| **O4** | **0.3446** | **0.4174** | **0.1600** | **0.01133** | **1** |
| **O5** | **0.1165** | **0.2379** | **0.1595** | **0.03141** | **1** |

Fig.S1. Gaussian fitting results of $Mn^{2+}$ emission band in NBB: $0.03Ce^{3+}$, $0.03Mn^{2+}$ (a); Mn1 and Mn2 shift evolution over the content of $Mn^{2+}$ in NBB: $0.03Ce^{3+}$, $yMn^{2+}$ (b).

Table S3. The atomic coordinates, site occupancies and temperature factors of $NB_{0.6}S_{0.4}B$: $0.03Ce^{3+}$, $0.03Mn^{2+}$ samples

| Atoms | x | y | z | Usio | Occupy |
|---|---|---|---|---|---|
| **Ba** | **0** | **0** | **0.0054** | **0.03130** | **1** |
| **Na** | **0** | **0** | **0.2280** | **0.04693** | **1** |
| **B1** | **0.3522** | **0.2657** | **0.0696** | **0.05631** | **1** |
| **B2** | **0.4673** | **0.3693** | **0.1591** | **0.03521** | **1** |
| **B3** | **0.2343** | **0.3656** | **0.1254** | **0.01630** | **1** |

| | | | | | |
|---|---|---|---|---|---|
| **O1** | **0.5011** | **0.3491** | **0.1163** | **0.02973** | **1** |
| **O2** | **0.2144** | **0.2387** | **0.0835** | **0.02251** | **1** |
| **O3** | **0.2106** | **0.4491** | **0.0772** | **0.01336** | **1** |
| **O4** | **0.3528** | **0.4087** | **0.1694** | **0.02355** | **1** |
| **O5** | **0.1095** | **0.2557** | **0.1614** | **0.03748** | **1** |

Table S4. Cell parameters (a/b, c) and volume (V) of $NB_{1-z}S_zB$: $0.03Ce^{3+}$

| z | a=b | c | V | Rp | Rwp | χ2 |
|---|---|---|---|---|---|---|
| 0 | 11.102 | 17.392 | 1856.56 | 6.78% | 8.99% | 2.67 |
| 0.1 | 11.091 | 17.401 | 1853.81 | 6.38% | 8.34% | 2.27 |
| 0.2 | 11.074 | 17.424 | 1850.51 | 7.48% | 9.80% | 2.55 |
| 0.3 | 11.055 | 17.455 | 1846.85 | 8.05% | 10.53% | 3.67 |
| 0.4 | 11.029 | 17.495 | 1842.88 | 8.74% | 11.48% | 4.56 |

Table S5. The atomic coordinates, site occupancies and temperature factors of $NB_{0.7}S_{0.3}B$: $0.03Ce^{3+}$ samples

| Atoms | x | y | z | Usio | Occupy |
|---|---|---|---|---|---|
| Ba | 0 | 0 | 0.0043 | 0.02613 | 1 |
| Na | 0 | 0 | 0.2244 | 0.03509 | 1 |
| B1 | 0.3796 | 0.2459 | 0.0602 | 0.03782 | 1 |
| B2 | 0.4467 | 0.3670 | 0.1821 | 0.02881 | 1 |
| B3 | 0.2199 | 0.3210 | 0.1254 | 0.00721 | 1 |
| O1 | 0.4947 | 0.3431 | 0.1146 | 0.02805 | 1 |
| O2 | 0.2295 | 0.2339 | 0.0650 | 0.00681 | 1 |

| | | | | | |
|---|---|---|---|---|---|
| **O3** | **0.2022** | **0.4242** | **0.0653** | **0.06140** | **1** |
| **O4** | **0.3439** | **0.4116** | **0.1643** | **0.04948** | **1** |
| **O5** | **0.1064** | **0.2502** | **0.1653** | **0.00616** | **1** |

Fig. S2. Emission spectra of $NB_{1-z}S_zB$: $0.03Ce^{3+}$ and emission intensity of $Ce^{3+}$ as a function of $Sr^{2+}$ content (a); Rietveld refinement results of $NB_{0.7}S_{0.3}B$: $0.03Ce^{3+}$ (b).

Fig.S3. Decay curves and lifetimes of $Ce^{3+}$, Mn1 and Mn2 in $NB_{0.6}S_{0.4}B$: $0.03Ce^{3+}$, $0.03Mn^{2+}$ at different temperature.