

Supporting Information

Development of cyan blue-emitting Ba₃La₂(BO₃)₄:Ce³⁺,Tb³⁺ phosphor for use in dental glassing materials: color tunable emission and energy transfer

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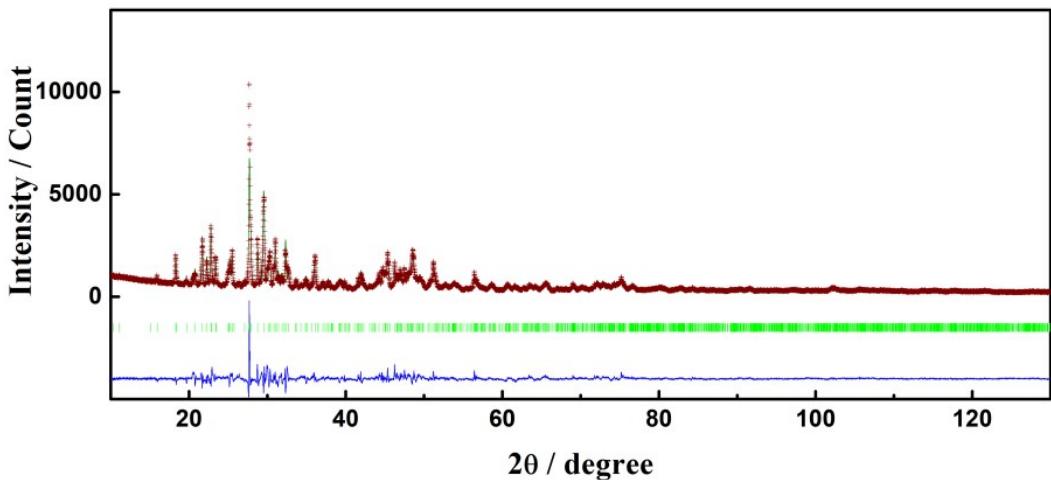


Figure S1. Rietveld refinement result for X-ray powder diffraction data of $\text{Ba}_3\text{La}_2(\text{BO}_3)_4:0.05\text{Ce}^{3+}$. Red symbol: measured pattern, green solid line: calculated pattern, blue solid line: difference between their intensities.

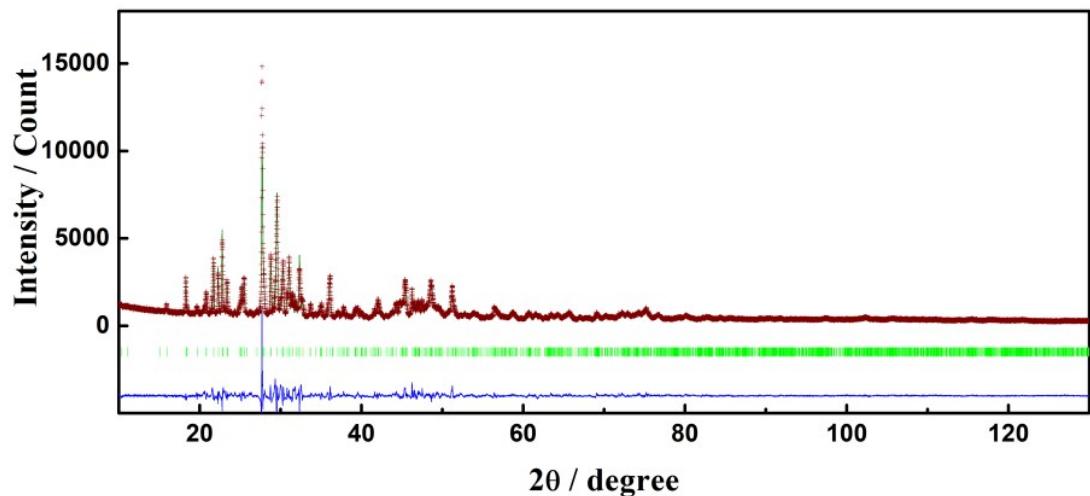


Figure S2. Rietveld refinement result for X-ray powder diffraction data of $\text{Ba}_3\text{La}_2(\text{BO}_3)_4:0.03\text{Tb}^{3+}$. Red symbol: measured pattern, green solid line: calculated pattern, blue solid line: difference between their intensities.

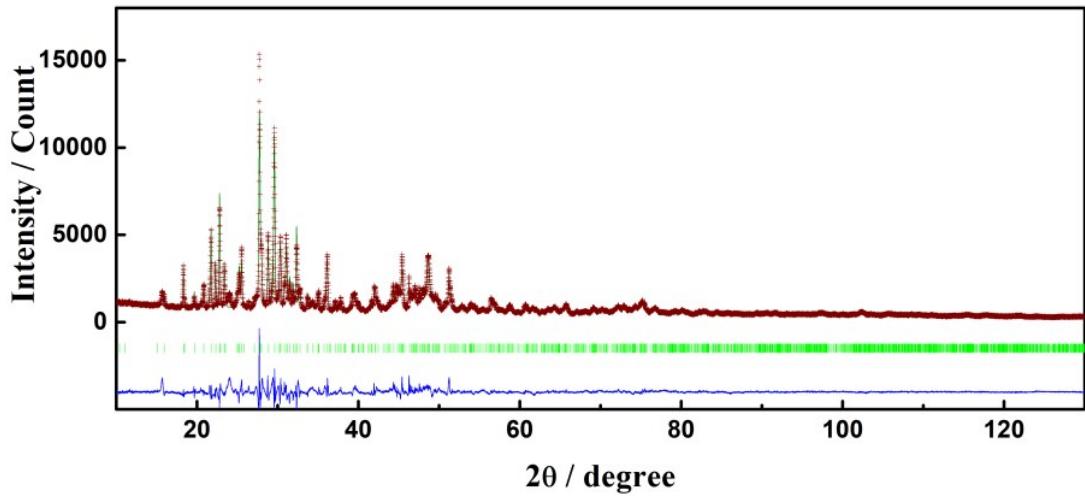


Figure S3. Rietveld refinement result for X-ray powder diffraction data of $\text{Ba}_3\text{La}_2(\text{BO}_3)_4:0.05\text{Ce}^{3+},0.03\text{Tb}^{3+}$. Red symbol: measured pattern, green solid line: calculated pattern, blue solid line: difference between their intensities.

Table S1. Refined structural parameters of the $\text{Ba}_3\text{La}_2(\text{BO}_3)_4$ host material from the Rietveld refinement using XRD data obtained at room temperature.

| Atom | Site | Occ. | <i>x</i> | <i>y</i> | <i>z</i> | Beq |
|------|-----------|------|-----------|-----------|-----------|-----|
| La1 | <i>4c</i> | 0.67 | 0.3113(7) | 0.25 | 0.5299(5) | 1.0 |
| Ba1 | <i>4c</i> | 0.33 | 0.3113(7) | 0.25 | 0.5299(5) | 1.0 |
| La2 | <i>8d</i> | 0.33 | 0.1828(3) | 0.1250(2) | 0.1493(1) | 1.0 |
| Ba2 | <i>8d</i> | 0.67 | 0.1828(3) | 0.1250(2) | 0.1493(1) | 1.0 |
| La3 | <i>8d</i> | 0.33 | 0.4813(6) | 0.5825(5) | 0.1769(3) | 1.0 |
| Ba3 | <i>8d</i> | 0.67 | 0.4813(6) | 0.5825(5) | 0.1769(3) | 1.0 |
| B1 | <i>4c</i> | 1 | 0.6473(5) | 0.25 | 0.1616(9) | 1.0 |
| B2 | <i>4c</i> | 1 | 0.4140(7) | 0.75 | 0.3093(1) | 1.0 |
| B3 | <i>8d</i> | 1 | 0.3216(0) | 0.4167(6) | 0.4138(6) | 1.0 |
| O1 | <i>8d</i> | 1 | 0.5466(1) | 0.3100(3) | 0.0909(8) | 1.0 |
| O2 | <i>4c</i> | 1 | 0.3613(5) | 0.25 | 0.2450(9) | 1.0 |
| O3 | <i>4c</i> | 1 | 0.6470(2) | 0.25 | 0.5304(5) | 1.0 |
| O4 | <i>8d</i> | 1 | 0.7525(8) | 0.6804(8) | 0.1845(0) | 1.0 |
| O5 | <i>8d</i> | 1 | 0.6658(1) | 0.6165(8) | 0.4068(8) | 1.0 |
| O6 | <i>8d</i> | 1 | 0.2377(9) | 0.4967(4) | 0.9932(4) | 1.0 |
| O7 | <i>8d</i> | 1 | 0.3546(1) | 0.4579(0) | 0.3369(2) | 1.0 |

Table S2. Refined structural parameters of the $\text{Ba}_3\text{La}_2(\text{BO}_3)_4:0.05\text{Ce}^{3+}$ phosphor from the Rietveld refinement using XRD data obtained at room temperature.

| Atom | Site | Occ. | <i>x</i> | <i>y</i> | <i>z</i> | Beq |
|------|-----------|------|-----------|-----------|-----------|-----|
| La1 | <i>4c</i> | 0.62 | 0.3104(8) | 0.25 | 0.5340(3) | 1.0 |
| Ba1 | <i>4c</i> | 0.33 | 0.3104(8) | 0.25 | 0.5340(3) | 1.0 |
| Ce1 | <i>4c</i> | 0.05 | 0.3104(8) | 0.25 | 0.5340(3) | 1.0 |
| La2 | <i>8d</i> | 0.28 | 0.1809(8) | 0.1268(6) | 0.1526(8) | 1.0 |
| Ba2 | <i>8d</i> | 0.67 | 0.1809(8) | 0.1268(6) | 0.1526(8) | 1.0 |
| Ce2 | <i>4c</i> | 0.05 | 0.1809(8) | 0.1268(6) | 0.1526(8) | 1.0 |
| La3 | <i>8d</i> | 0.28 | 0.4809(9) | 0.5816(3) | 0.1760(0) | 1.0 |
| Ba3 | <i>8d</i> | 0.67 | 0.4809(9) | 0.5816(3) | 0.1760(0) | 1.0 |
| Ce3 | <i>4c</i> | 0.05 | 0.4809(9) | 0.5816(3) | 0.1760(0) | 1.0 |
| B1 | <i>4c</i> | 1 | 0.6268(5) | 0.25 | 0.1571(4) | 1.0 |
| B2 | <i>4c</i> | 1 | 0.4143(0) | 0.75 | 0.3325(0) | 1.0 |
| B3 | <i>8d</i> | 1 | 0.3276(5) | 0.4839(8) | 0.4198(3) | 1.0 |
| O1 | <i>8d</i> | 1 | 0.5978(7) | 0.3236(4) | 0.0896(6) | 1.0 |
| O2 | <i>4c</i> | 1 | 0.3787(6) | 0.25 | 0.2266(5) | 1.0 |
| O3 | <i>4c</i> | 1 | 0.6734(5) | 0.25 | 0.5190(5) | 1.0 |
| O4 | <i>8d</i> | 1 | 0.7310(5) | 0.6880(9) | 0.1817(3) | 1.0 |
| O5 | <i>8d</i> | 1 | 0.6649(8) | 0.6236(8) | 0.4164(7) | 1.0 |
| O6 | <i>8d</i> | 1 | 0.2675(0) | 0.4915(4) | 1.0030(1) | 1.0 |
| O7 | <i>8d</i> | 1 | 0.3486(6) | 0.4610(6) | 0.3347(7) | 1.0 |

Table S3. Refined structural parameters of the $\text{Ba}_3\text{La}_2(\text{BO}_3)_4:0.03\text{Tb}^{3+}$ phosphor from the Rietveld refinement using XRD data obtained at room temperature.

| Atom | Site | Occ. | <i>x</i> | <i>y</i> | <i>z</i> | Beq |
|------|-----------|------|-----------|-----------|-----------|-----|
| La1 | <i>4c</i> | 0.62 | 0.3068(1) | 0.25 | 0.5291(5) | 1.0 |
| Ba1 | <i>4c</i> | 0.33 | 0.3068(1) | 0.25 | 0.5291(5) | 1.0 |
| Tb1 | <i>4c</i> | 0.05 | 0.3068(1) | 0.25 | 0.5291(5) | 1.0 |
| La2 | <i>8d</i> | 0.28 | 0.1818(0) | 0.1250(0) | 0.1503(1) | 1.0 |
| Ba2 | <i>8d</i> | 0.67 | 0.1818(0) | 0.1250(0) | 0.1503(1) | 1.0 |
| Tb2 | <i>4c</i> | 0.05 | 0.1818(0) | 0.1250(0) | 0.1503(1) | 1.0 |
| La3 | <i>8d</i> | 0.28 | 0.4802(1) | 0.5837(7) | 0.1763(8) | 1.0 |
| Ba3 | <i>8d</i> | 0.67 | 0.4802(1) | 0.5837(7) | 0.1763(8) | 1.0 |
| Tb3 | <i>4c</i> | 0.05 | 0.4802(1) | 0.5837(7) | 0.1763(8) | 1.0 |
| B1 | <i>4c</i> | 1 | 0.4548(4) | 0.25 | 0.0868(2) | 1.0 |
| B2 | <i>4c</i> | 1 | 0.3802(8) | 0.75 | 0.4089(2) | 1.0 |
| B3 | <i>8d</i> | 1 | 0.2815(4) | 0.4528(5) | 0.4142(5) | 1.0 |
| O1 | <i>8d</i> | 1 | 0.6002(9) | 0.3135(9) | 0.1019(7) | 1.0 |
| O2 | <i>4c</i> | 1 | 0.3812(1) | 0.25 | 0.2269(0) | 1.0 |
| O3 | <i>4c</i> | 1 | 0.6476(5) | 0.25 | 0.5383(3) | 1.0 |
| O4 | <i>8d</i> | 1 | 0.7651(2) | 0.6877(5) | 0.1805(7) | 1.0 |
| O5 | <i>8d</i> | 1 | 0.6649(7) | 0.6230(6) | 0.4032(7) | 1.0 |
| O6 | <i>8d</i> | 1 | 0.2786(7) | 0.4944(9) | 0.9956(8) | 1.0 |
| O7 | <i>8d</i> | 1 | 0.3749(4) | 0.4537(8) | 0.3384(7) | 1.0 |

Table S4. Refined structural parameters of the $\text{Ba}_3\text{La}_2(\text{BO}_3)_4:0.05\text{Ce}^{3+}, 0.03\text{Tb}^{3+}$ phosphor from the Rietveld refinement using XRD data obtained at room temperature.

| Atom | Site | Occ. | <i>x</i> | <i>y</i> | <i>z</i> | Beq |
|------|-----------|------|-----------|-----------|-----------|-----|
| La1 | <i>4c</i> | 0.59 | 0.3054(9) | 0.25 | 0.5337(3) | 1.0 |
| Ba1 | <i>4c</i> | 0.33 | 0.3054(9) | 0.25 | 0.5337(3) | 1.0 |
| Ce1 | <i>4c</i> | 0.05 | 0.3054(9) | 0.25 | 0.5337(3) | 1.0 |
| Tb1 | <i>4c</i> | 0.03 | 0.3054(9) | 0.25 | 0.5337(3) | 1.0 |
| La2 | <i>8d</i> | 0.25 | 0.1842(8) | 0.1260(6) | 0.1541(0) | 1.0 |
| Ba2 | <i>8d</i> | 0.67 | 0.1842(8) | 0.1260(6) | 0.1541(0) | 1.0 |
| Ce2 | <i>4c</i> | 0.05 | 0.1842(8) | 0.1260(6) | 0.1541(0) | 1.0 |
| Tb2 | <i>4c</i> | 0.03 | 0.1842(8) | 0.1260(6) | 0.1541(0) | 1.0 |
| La3 | <i>8d</i> | 0.25 | 0.4794(3) | 0.5830(4) | 0.1778(7) | 1.0 |
| Ba3 | <i>8d</i> | 0.67 | 0.4794(3) | 0.5830(4) | 0.1778(7) | 1.0 |
| Ce3 | <i>4c</i> | 0.05 | 0.4794(3) | 0.5830(4) | 0.1778(7) | 1.0 |
| Tb3 | <i>4c</i> | 0.03 | 0.4794(3) | 0.5830(4) | 0.1778(7) | 1.0 |
| B1 | <i>4c</i> | 1 | 0.6405(1) | 0.25 | 0.1472(1) | 1.0 |
| B2 | <i>4c</i> | 1 | 0.3929(6) | 0.75 | 0.3855(0) | 1.0 |
| B3 | <i>8d</i> | 1 | 0.2665(8) | 0.4911(5) | 0.4303(5) | 1.0 |
| O1 | <i>8d</i> | 1 | 0.5964(7) | 0.3235(0) | 0.0868(8) | 1.0 |
| O2 | <i>4c</i> | 1 | 0.4057(7) | 0.25 | 0.2249(1) | 1.0 |
| O3 | <i>4c</i> | 1 | 0.6575(9) | 0.25 | 0.5172(0) | 1.0 |
| O4 | <i>8d</i> | 1 | 0.7411(6) | 0.6944(0) | 0.2060(5) | 1.0 |
| O5 | <i>8d</i> | 1 | 0.6530(7) | 0.6097(0) | 0.4441(8) | 1.0 |
| O6 | <i>8d</i> | 1 | 0.2716(7) | 0.4910(8) | 1.0159(3) | 1.0 |
| O7 | <i>8d</i> | 1 | 0.3720(2) | 0.4620(7) | 0.3480(3) | 1.0 |

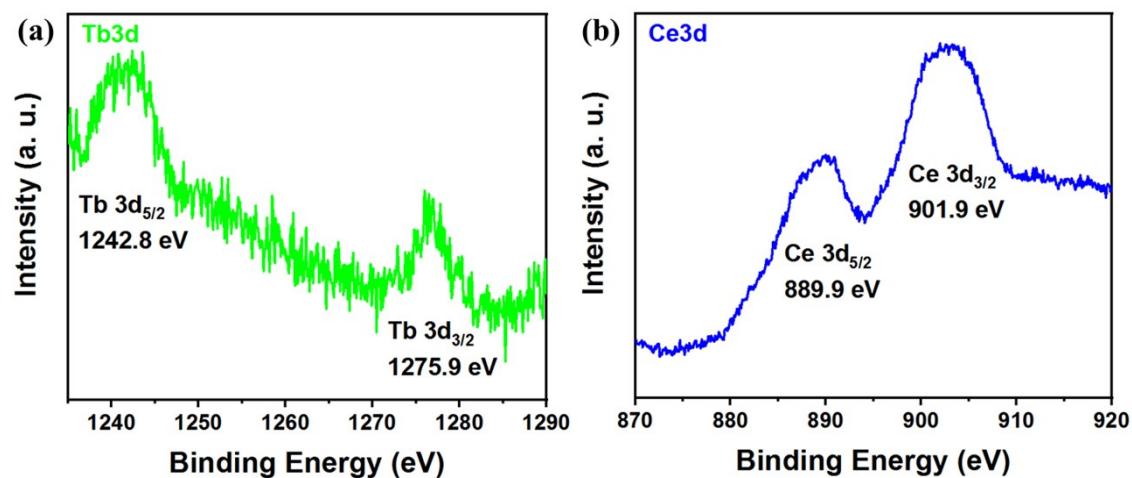


Figure S4. The (a) Ce3d and (b) Tb3d XPS spectra of $\text{Ba}_3\text{La}_2(\text{BO}_3)_4:0.05\text{Ce}^{3+},0.13\text{Tb}^{3+}$ phosphor.