Electronic Supplementary Information (ESI) for

Near Ultraviolet Excitable Cyan-Green Phosphors of $Ba_6La_2Al_3ScO_{15}:Ce^{3+}$ and $Ba_6La_2Al_3ScO_{15}:Ce^{3+},Tb^{3+}$: Investigations on Crystal Structure, Site Assignment of Ce^{3+} and Tb^{3+} ions, and Energy Transfer Process from Ce^{3+} to Tb^{3+}

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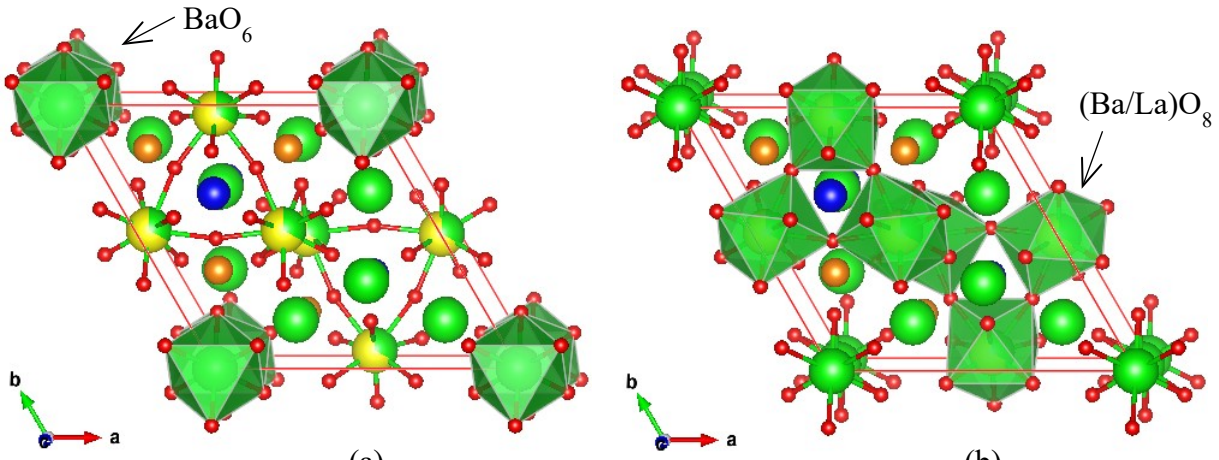

Figure S1. (a) Linkage of BaO_6 octahedra along [001] direction and (b) network of $(Ba/La)O_8$ polyhedra.

Table S1a. Bond distances(Å) and polyhedral indices of BaO_6 polyhedron in BLASO.

Ba1 - O4	2.586(12)
Ba1 - O4	2.892(13)
Ba1 - O4	2.892(13)
Ba1 - O4	2.586(12)
Ba1 - O4	2.586(12)
Ba1 - O4	2.892(13)
Average bond length	2.7394 Å
Polyhedral volume	26.5229 $Å^3$
Distortion index(bond length)	0.05586
Effective coordination number	5.2062

Table S1b. Bond distances(Å) and polyhedral indices of$(Ba/La)O_8$ polyhedron in BLASO.

Ba4/La4 - O2	2.636(7)
Ba4/La4 - O1	2.691(10)
Ba4/La4 - O3	2.73(2)
Ba4/La4 - O1	2.499(10)
Ba4/La4 - O2	2.636(7)
Ba4/La4 - O1	2.691(10)
Ba4/La4 - O3	2.381(14)
Ba4/La4 - O1	2.499(10)
Average bond length	2.5948 Å
Polyhedral volume	30.4526 $Å^3$
Distortion index(bond length)	0.03912
Effective coordination number	7.1312

Table S1c. Bond distances(Å) and polyhedral indices of BaO_{10} polyhedron in BLASO.

Ba2 - O1	2.856(12)
Ba2 - O4	3.099(7)
Ba2 - O3	2.903(6)
Ba2 - O1	3.144(9)
Ba2 - O4	3.184(14)
Ba2 - O2	2.666(19)
Ba2 - O1	3.144(9)
Ba2 - O4	3.099(7)
Ba2 - O3	2.903(6)
Ba2 - O1	2.856(12)
Average bond length	2.9853 Å
Polyhedral volume	56.5525 $Å^3$
Distortion index(bond length)	0.04974
Effective coordination number	8.1618

Table S1d. Bond distances(Å) and polyhedral indices of BaO_{12} polyhedron in BLASO.

Ba3 - O1	3.219(13)
Ba3 - O1	3.219(13)
Ba3 - O2	3.271(19)
Ba3 - O3	2.768(19)
Ba3 - O3	2.768(19)
Ba3 - O1	3.219(13)
Ba3 - O2	3.271(19)
Ba3 - O1	3.219(13)
Ba3 - O2	3.271(19)
Ba3 - O1	3.219(13)
Ba3 - O3	2.768(19)
Ba3 - O1	3.219(13)
Average bond length	3.1193 Å
Polyhedral volume	69.9772 $Å^3$
Distortion index(bond length)	0.05631
Effective coordination number	8.3884

Table S1e. Bond distances(Å) and polyhedral indices of YO_8 polyhedron in YAG.

Y1-O1	2.317(4)
Y1-O1	2.317(4)
Y1-O1	2.437(4)
Y1-O1	2.437(4)
Y1-O1	2.437(4)
Y1-O1	2.317(4)
Y1-O1	2.317(4)
Y1-O1	2.437(4)
Average bond length	2.3767 Å
Polyhedral volume	22.9811 $Å^3$
Distortion index(bond length)	0.02520
Effective coordination number	7.8058

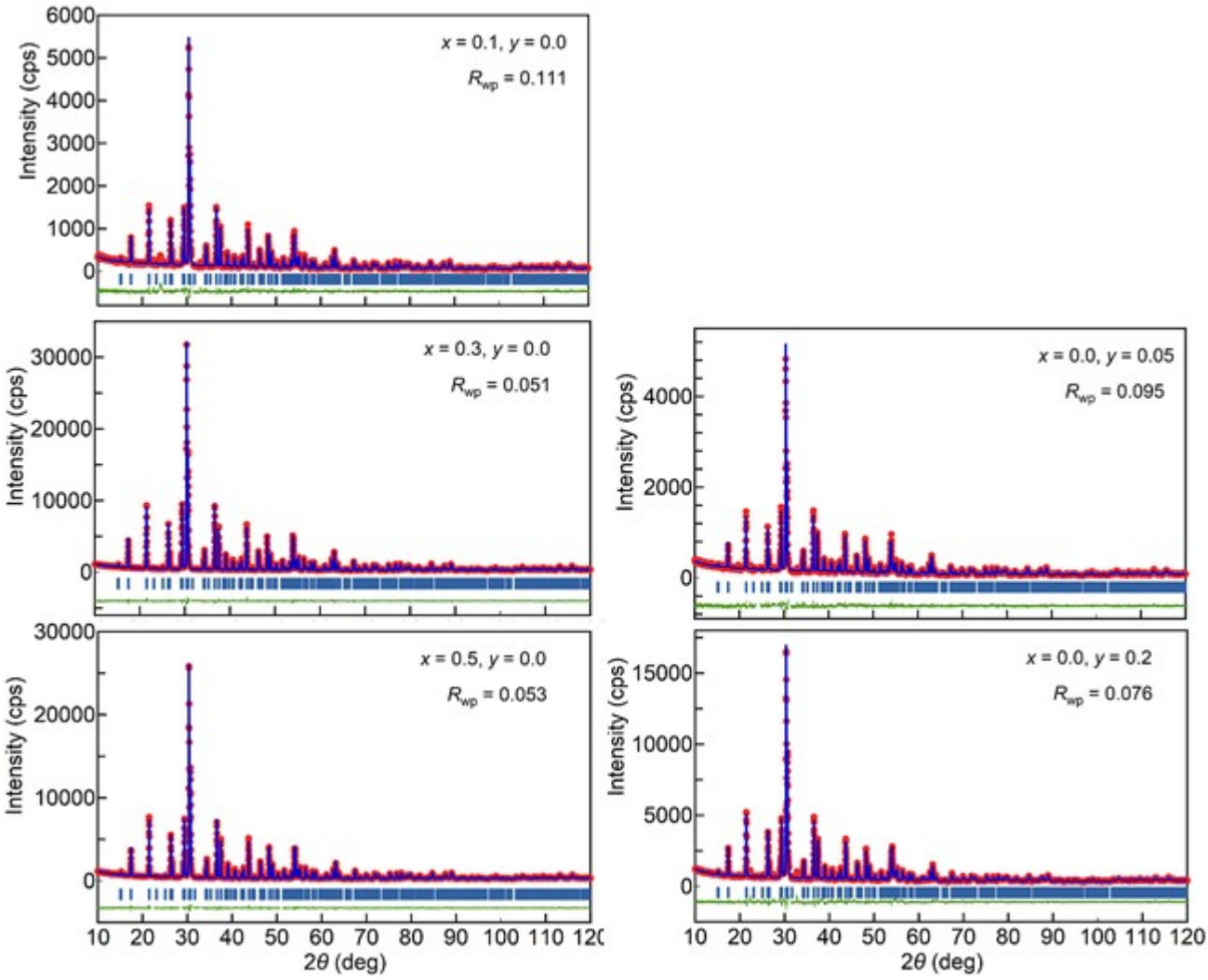

Figure S2. Powder pattern fitting of Rietveld refinement for $Ba_6La_{2(1-x-y)}Ce_{2x}Tb_{2y}Al_3ScO_{15}$. The species of Ce and Tb were not included in the refinement because their atomic numbers are close to that of Ba, providing no accurate occupancy factors.

The reliable factors in the Rietveld refinement

$$R_{wp} = \left[\frac{\sum_i w_i |y_i - f_i(a)|^2}{\sum_i w_i y_i^2}\right]^{1/2} \qquad (S1)$$

$$R_p = \frac{\sum_i |y_i - f_i(a)|}{\sum_i y_i} \qquad (S2)$$

$$R_B = \frac{\sum_K |I_{obs}(h_K) - I_{cal}(h_K)|}{\sum_K I_{obs}(h_K)} \qquad (S3)$$

$$R_F = \frac{\sum_K ||F_{obs}(h_K)| - |F_{cal}(h_K)||}{\sum_K |F_{obs}(h_K)|} \qquad (S4)$$

$$R_e = \left[\frac{m-n}{\sum_i w_i y_i^2}\right]^{1/2} \qquad (S5)$$

$$S = \frac{R_{wp}}{R_e} = \left(\frac{\sum_i w_i |y_i - f_i(a)|^2}{m-n}\right)^{1/2} \qquad (S6)$$

Where m is the number of steps in the step-scan measurement, $I_{obs}(h_K)$ and $I_{cal}(h_K)$ theobserved and calculated integral intensity for Blagg reflection K, respectively, and $F_{obs}(h_K)$ and $F_{cal}(h_K)$ the observed and calculated structure factures, repectively.

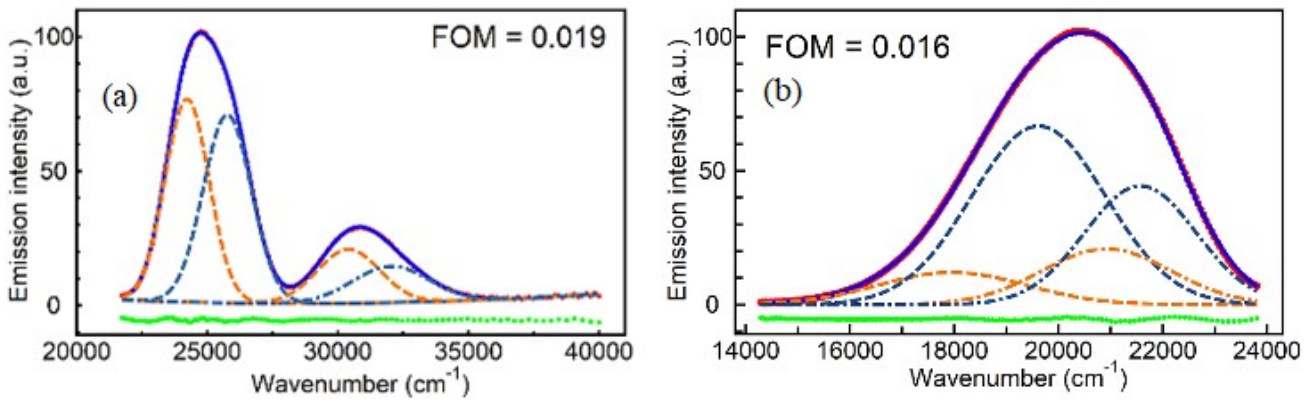

Figure S3. The actual deconvolution in the cm^{-1} unit for (a) excitation (b) emission curves. The index of FOM is the Figure-of-merit defined in equation S7.

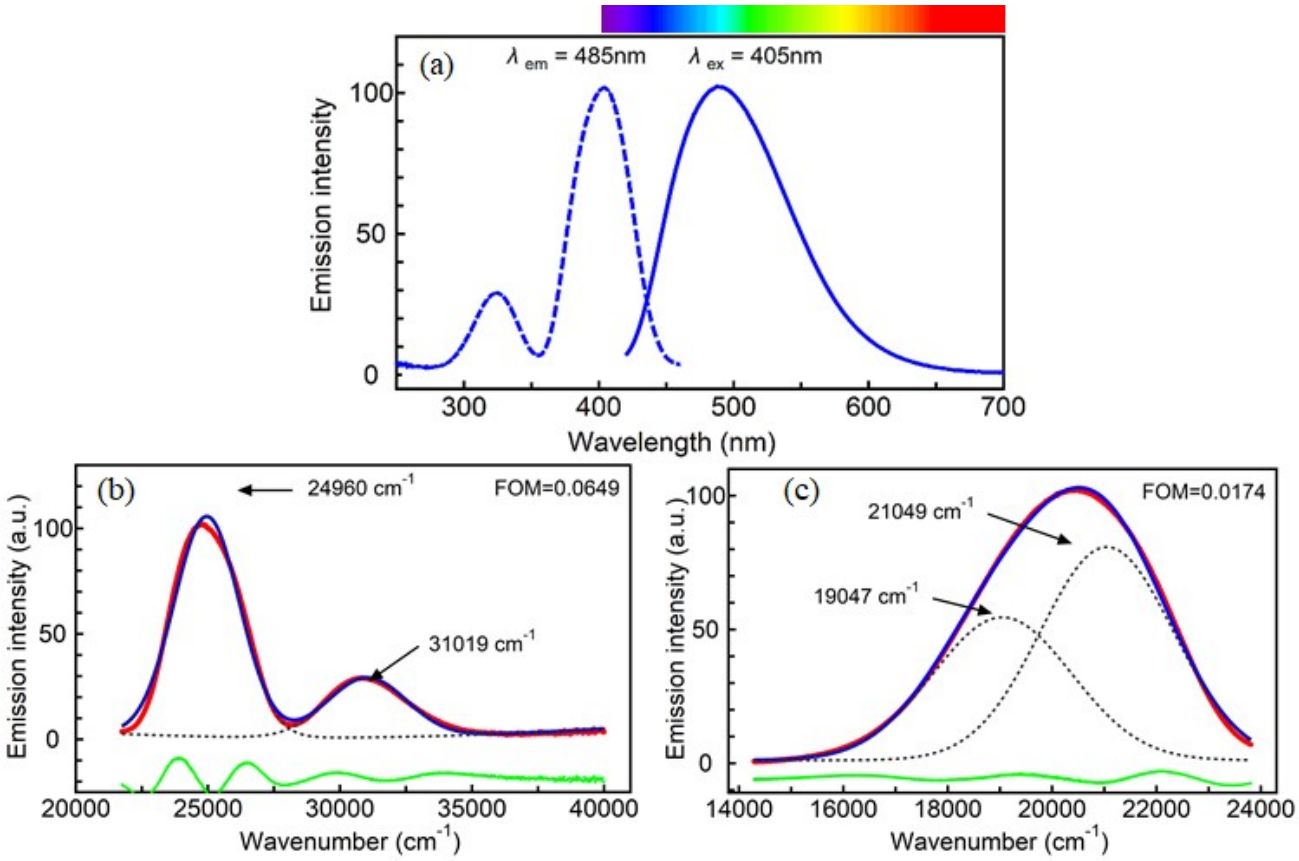

Figure S4. (a) Excitation (dashed line) and emission (solid) spectra of BLASO:Ce^{3+}(x = 0.015) and Gaussian fitting of (b) excitation and (c) emission of BLASO:Ce^{3+} by two components.

Index of FOM

It is defined as,

$$FOM = \left[\frac{\sum_i w_i \left|y_i^{obs} - y_i^{cal}\right|^2}{\sum_i w_i y_i^{obs2}}\right]^{1/2} \qquad (S7)$$

where y_i^{obs} is the intensity at ith data, y_i^{cal} the intensity at ith data calculated from the model Gaussian function and w_i the weighting factor at ith data, usually all factors set to 1.

Calculation of Dorenbos model

The total energy shift from the lowest 5d level edge in a compound A, $E_{total}(Ce^{3+},A)$, can be described as equation 1,[1-2]

$$E_{total}(Ce^{3+},A) = 49{,}340\ cm^{-1} - \varepsilon_C - \varepsilon_{cfs} - \Delta S(A) \quad (S8)$$

where the value of $49340\ cm^{-1}$ is the energy of free Ce^{3+}, ε_C means the centroid shift, ε_{cfs} is the crystal field splitting, $\Delta S(A)$ is the Stokes shift estimated from the excitation and emission spectra of compound A. The centroid shift ε_C is estimated from the following equation,[3-4]

$$\varepsilon_C = 1.79 \times 10^{13} \sum_{i=1}^{N} \frac{\alpha_{sp}^{i}}{(R_i - 0.6\Delta R)^6} \quad (S9)$$

where R_i represents the bond distance of the Ce^{3+}-O^{2-} ions in the host lattice, ΔR is the difference in the ionic radii between Ce^{3+} and the host cation replaced by Ce^{3+} (Ba^{2+} and La^{3+} in this case), N is the number of anions coordinated with Ce^{3+}, and α_{sp}^{i} the spectroscopic polarizability, which is described as,[4]

$$\alpha_{sp}^{i} = 0.33 + \frac{4.8}{\chi_{av}^{2}} \quad (S10)$$

where χ_{av} is the weighted average of the cation electronegativity in s host lattice. The strength of the crystal field splitting, ε_{cfs}, for a polyhedron can be estimated from the following equation,[4]

$$\varepsilon_{cfs} = \beta_{poly}^{Q} R_{av}^{-2} \quad (S11)$$

where β_{poly}^{Q} has a constant dependent on the shape and coordination number, and R_{av} the average bond distance of the polyhedron, which is defined as,[4]

$$R_{av} = \frac{1}{N} \sum_{i=1}^{N} (R_i - 0.6\Delta R) \quad (S12)$$

where R_i is the bond distance between Ce^{3+} and N number of coordinating anions, and ΔR the difference in ionic radii between the central cation and Ce^{3+}. The experimentally determined Stokes shift value of 4100 cm^{-1}, estimated from the single component fitting in Figure S4, is used in the calculation. The value are comparable to that of γ-Ca_2SiO_4:Ce^{3+} (4560 cm^{-1})[5] and a little larger than those of YAG: Ce^{3+} (~2700 cm^{-1}),[6] Sr_3GaO_4F:Ce^{3+} (2762 cm-1)[7] and $Lu_2CaMg_2Si_3O_{12}$: Ce^{3+} (2550 cm^{-1})[8] phosphors.

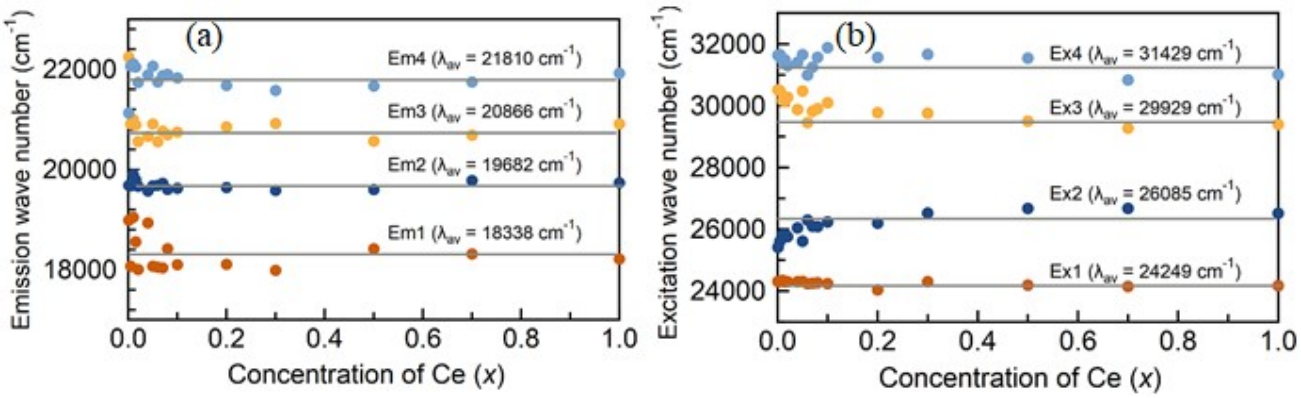

Figure S5. Concentration dependence of (a) emission and (b) excitation wave numbers on Ce in BLASO:Ce^{3+}.

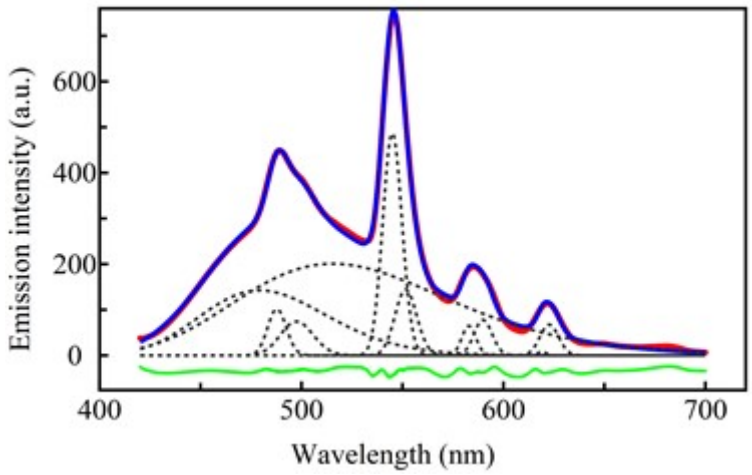

Figure S6. Deconvolution of emission band of BLASO:Ce^{3+}(x = 0.015),Tb^{3+}(y = 0.05) using Gaussian Function.

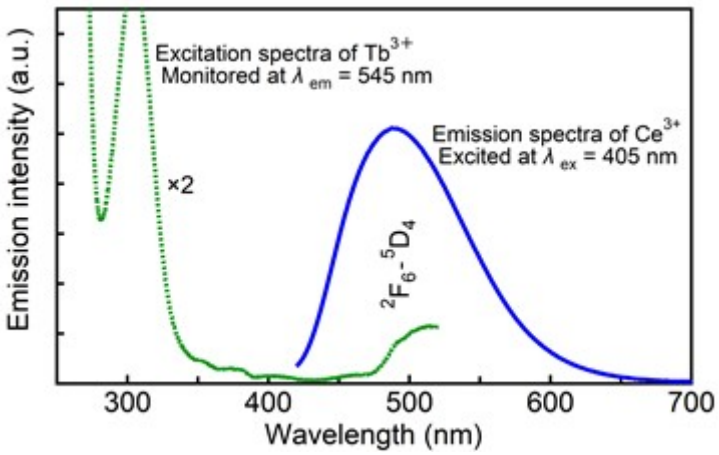

Figure S7. Overlap between excitation of Tb^{3+} (green dashed line) and emission of Ce^{3+} (blue solid line) in BLASO.

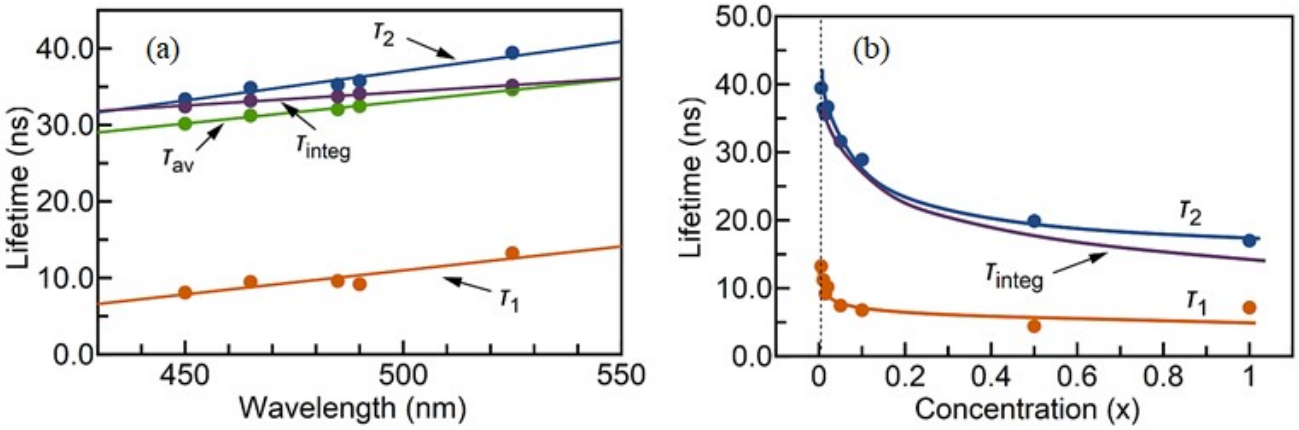

Figure S8. (a) Dependence of Ce^{3+} lifetimes on emission wavelength and (b) concentration of Ce^{3+}.

Table S2. The values of a_1, a_2, and b_1 in Martin model equation.

s	a_1	a_2	b_1
6	10.866	15.500	8.743
8	17.072	35.860	13.882
10	24.524	67.909	20.290

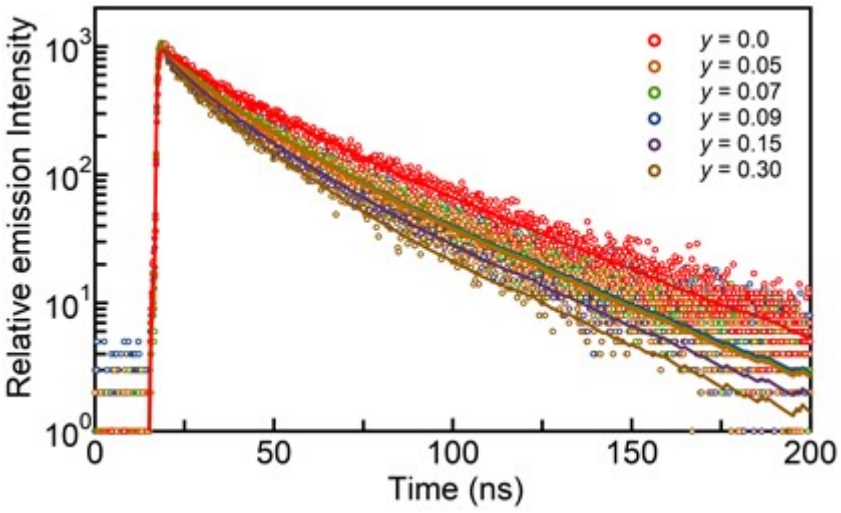

Figure S9. Results of decay curve fitting to Yokota-Tanimoto equation for BLASO:Ce^{3+}(x = 0.015),Tb^{3+}(y = 0.05 - 0.30).

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