A non-concentration-quenching phosphor $Ca_3Eu_2B_4O_{12}$ for WLED application

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Table S1 Crystallographic data, structure refinement parameters of CYBO: $0.15Eu^{3+}$

Formula	$Ca_3Y_{1.85}Eu_{0.15}B_4O_{12}$
Crystal system	orthorhombic
Space group	P n m a (62)
a, b, c (Å)	7.1644(4), 15.4729(9), 8.5573(5)
α, β, γ (°)	90, 90, 90
Volume(Å^3)	948.61(9)
Z, $\rho_{calc.}$(g cm^{-3})	4, 3.7966
Sample	Multi-crystal powder
Radiation type	Cu Kα
2θ range (°)	5.0080 - 129.9750
Step size	0.017
No. of refined parameters	124
R_B (%)	7.48
R_P (%)	2.53
R_{WP} (%)	3.66
S	2.18

Table S2 Atomic coordinate, thermal vibration parameter, Wyckoff position, and occupancy for CYBO: $0.15Eu^{3+}$

Atom	x/a	y/b	z/c	Uiso	Site.	Occ
Ca1	0.3237(4)	0.25	0.5326(3)	0.0014	4c	0.252
Y1	0.3237(4)	0.25	0.5326(3)	0.0014	4c	0.692
Eu1	0.3237(4)	0.25	0.5326(3)	0.0014	4c	0.056
Y2	0.1939(5)	0.1277(2)	0.1554(4)	0.0038	8d	0.139
Eu2	0.1939(5)	0.1277 (2)	0.1554(4)	0.0038	8d	0.011
Ca2	0.1939(5)	0.1277(2)	0.1554(4)	0.0038	8d	0.850
Y3	0.4792(4)	0.5838(2)	0.1757(3)	0.0045	8d	0.440
Eu3	0.4792(4)	0.5838(2)	0.1757(3)	0.0045	8d	0.036
Ca3	0.4792(4)	0.5838(2)	0.1757(3)	0.0045	8d	0.524
B1	0.4900	0.25	0.2500	0.0063	4c	1
B2	0.2770	0.75	0.3560	0.0063	4c	1
B3	0.3280	0.4560	0.4510	0.0063	8d	1
O1	0.5452(1)	0.25	0.0704(1)	0.0063	8d	1
O2	0.3495(2)	0.25	0.2483 (2)	0.0063	4c	1
O3	0.6737(2)	0.25	0.5012(2)	0.0063	4c	1
O4	0.7659(2)	0.6803(5)	0.2265(1)	0.0063	8d	1
O5	0.6052(1)	0.5907(7)	0.4543(1)	0.0063	8d	1
O6	0.2825(1)	0.4776(6)	0.9907(1)	0.0063	8d	1
O7	0.3661(1)	0.4671(7)	0.2943(1)	0.0063	8d	1

Table S3 Bond distance and bond angle for CYBO: $0.15Eu^{3+}$

Bond		Symmetry Operation	Length (Å)
Y1|Ca1|Eu1	O4	1-x, 1-y, 1-z	2.4134(3)
	O4	1-x, -0.5+y, 1-z	2.4134(3)
	O2	x, y, z	2.4398(3)
	O1	-0.5+x, 0.5-y, 0.5-z	2.4674(3)
	O1	-0.5+x, y, 0.5-z	2.4674(3)
	O5	1-x, 1-y, 1-z	2.5195(1)
	O5	1-x, -0.5+y, 1-z	2.5195(1)
	O3	x, y, z	2.5219(3)
	Average		2.4365
Ca2|Y2|Eu2	O6	x, 0.5-y, -1+z	2.2460(3)
	O7	x, 0.5-y, z	2.2553(4)
	O3	-0.5+x, 0.5-y, 0.5-z	2.3230(3)
	O2	x, y, z	2.3354(3)
	O1	-0.5+x, 0.5-y, 0.5-z	2.6811(4)
	O1	x, 0.5-y, z	2.7219(4)
	O7	-0.5+x, 0.5-y, 0.5-z	2.8025(4)
	O5	0.5-x, -0.5+y, -0.5+z	2.8071(4)
	Average		2.5215
Ca3|Y3|Eu3	O7	x, y, z	2.2242(3)
	O4	-0.5+x, y, 0.5-z	2.2943(3)
	O6	1-x, 1-y, 1-z	2.4176(3)
	O1	1-x, 1-y, -z	2.5450(3)
	O5	x, y, z	2.5514(3)
	O4	x, y, z	2.5762(3)
	O6	x, y, -1+z	2.6816(3)
	Average		2.4701
B1	O1	x, 0.5-y, z	1.3056(9)
	O1	x, y, z	1.3056(9)
	O2	x, y, z	1.4584(1)
	Average		1.3565
B2	O3	1-x, 0.5+y, 1-z	1.2721(2)
	O4	-0.5+x, y, 0.5-z	1.2921(8)
	O4	-0.5+x, 1.5-y, 0.5-z	1.2921(8)
	Average		1.2854
B3	O5	1-x, 1-y, 1-z	1.1866(1)
	O6	0.5-x, 1-y, -0.5+z	1.3408(9)
	O7	x, y, z	1.3790(1)
	Average		1.3021

Table S4 Bond distance and bond angle for $Ca_3Eu_2B_4O_{12}$

Bond		Symmetry Operation	Length (Å)
Eu1|Ca1	O2	x, y, z	2.3304(8)
	O4	1-x, -0.5+y, 1-z	2.4167(7)
	O4	1-x, 1-y, 1-z	2.4167(7)
	O3	x, y, z	2.4279(1)
	O5	1-x, -0.5+y, 1-z	2.4430(7)
	O5	1-x, 1-y, 1-z	2.4430(7)
	O1	-0.5+x, y, 0.5-z	2.4521(7)
	O1	-0.5+x, 0.5-y, 0.5-z	2.4521(7)
	Average		2.4215
Ca2|Eu2	O6	x, 0.5-y, -1+z	2.3054(7)
	O7	x, 0.5-y, z	2.3572(7)
	O3	-0.5+x, 0.5-y, 0.5-z	2.371(5)
	O2	x, y, z	2.4855(6)
	O7	-0.5+x, 0.5-y, 0.5-z	2.5408(8)
	O1	-0.5+x, 0.5-y, 0.5-z	2.6927(7)
	O1	x, 0.5-y, z	2.7869(8)
	O5	0.5-x, -0.5+y, -0.5+z	2.8507(7)
	Average		2.5504
Ca3|Eu3	O7	x, y, z	2.3594(7)
	O4	x, y, z	2.3981(7)
	O6	1-x, 1-y, 1-z	2.4030(7)
	O4	-0.5+x, y, 0.5-z	2.4102(7)
	O5	x, y, z	2.5217(7)
	O1	1-x, 1-y, -z	2.5774(6)
	O6	x, y, -1+z	2.6092(7)
	Average		2.4685
B1	O2	x, y, z	1.3609(9)
	O1	x, 0.5-y, z	1.3685(6)
	O1	x, y, z	1.3685(6)
	Average		
B2	O3	1-x, 0.5+y, 1-z	1.3451(8)
	O4	-0.5+x, 1.5-y, 0.5-z	1.3560(6)
	O4	-0.5+x, y, 0.5-z	1.3560(6)
	Average		
B3	O6	0.5-x, 1-y, -0.5+z	1.3183(6)
	O5	1-x, 1-y, 1-z	1.3222(7)
	O7	x, y, z	1.3395(7)
	Average		

- Details for the calculation of quantum yield experiment

  Absorption rate and quantum yield are calculated as follows:

$$A = \frac{(L_b - L_c)}{L_b} \quad (1)$$

$$\emptyset_f = \frac{[E_c - (1 - A) \cdot E_b]}{L_b \cdot A} \quad (2)$$

Where A is the absorbance of the sample calculated by integrating the emission spectrum intensity; L_b is the scattering intensity of the surface of the integrating sphere obtained when the sample is not placed in the optical path; L_c is the scattering intensity of the surface of the integrating sphere when the detected sample is present; Φ_f is the quantum yield of the calculated sample; E_b is the luminescence intensity detected at the time of the sample not placed in the optical path; E_c is the emission intensity when the detected sample is present; L_a is the scattering of the integrating sphere itself.

Here, since the excitation light and the phosphor are not in the same optical path, L_b is equivalent to the scattering of the surface of the integrating sphere when no sample is placed. In this sense, L_b represents the scattering of the integrating sphere itself, i.e. $L_a = L_b$.

Quantum yield, which is commonly considered as the internal quantum efficiency, according to its physical definition:

QY= (Photons · Emitted) / (Photons · Absorbed) (3)

It means that the single “molecule” in the compound emits a photon after being excited by the light source, it is not "total emission photon/total absorption photon" in number, although in many cases the two are approximately equal. Combining the analysis of the emission spectrum intensity before, we have realized that the quantum yield is not equal to the emission spectrum intensity, that is, high quantum yield does not mean that the luminescence intensity is high, even though they are similar in some cases and have a consistent pattern. The definition of quantum yield refers to a single compound or molecule. Therefore, if the number of defects is large, the integrity of a single compound molecule is “destroyed”, and the quantum yield measured at this

time has not yet reached a maximum value, even if the luminescence intensity is the best among a given series of compounds. This also shows that the quantum yield is positively correlated with the crystallinity to a certain extent, which explains why the quantum yield can not only evaluate the sensitivity and interference degree of the fluorescent material to be measured, but also evaluate the purity of the material.