Nonstoichiometry as a hidden aspect of $TbAl_3(BO_3)_4$ optical properties

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Table S1. Summary data about the single crystal XRD data-collection parameters, structure refinement of crystals from batch II (Figure 1).

Chemical formula	$TbAl_3(BO_3)_4$
Temperature (K)	220
Cell setting	trigonal
Space group	*R*32
a (Å)	9.2986(2)
b (Å)	9.2986(2)
c (Å)	7.2542(2)
α(°)	90
β (°)	90
γ(°)	120
V (Å^3)	543.19(3)
Z	3
Calculated density, D_x (g cm^{-3})	4.357
Crystal size (mm)	0.18 × 0.09 × 0.03
Crystal form	plate
Data collection	
Diffractometer	Bruker D8 Venture diffractometer, Bruker PHOTON III area detector
Radiation; λ	MoK_α; 0.71073
Data range θ(°); *h*, *k*, *l*	–14< *h* < 14, –14 < *k* < 12, –11 < *l* < 11
No. of measured reflections	4817
Total reflections (N_2) / observed(N_1)	538
Criterion for observed reflections	$I > 3\sigma(I)$
R_{int} (%)	5.05
Refinement	
R_1, wR_1 [$I > 3\sigma(I)$]	0.0094
R_1, wR_1 [all]	0.0219
GooF (Goodness of fit)	1.1

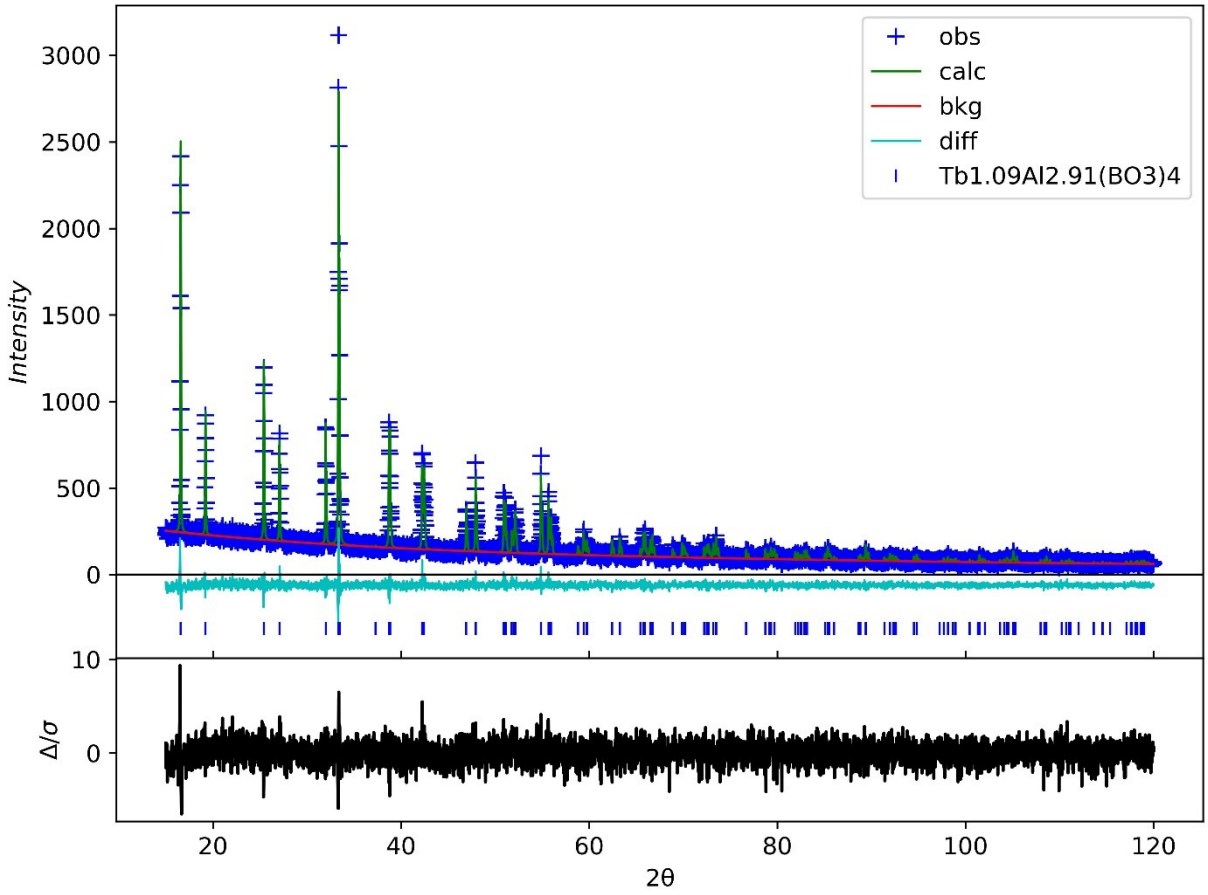

Figure S1. Rietveld plot of the sample from batch II (Figure 1).

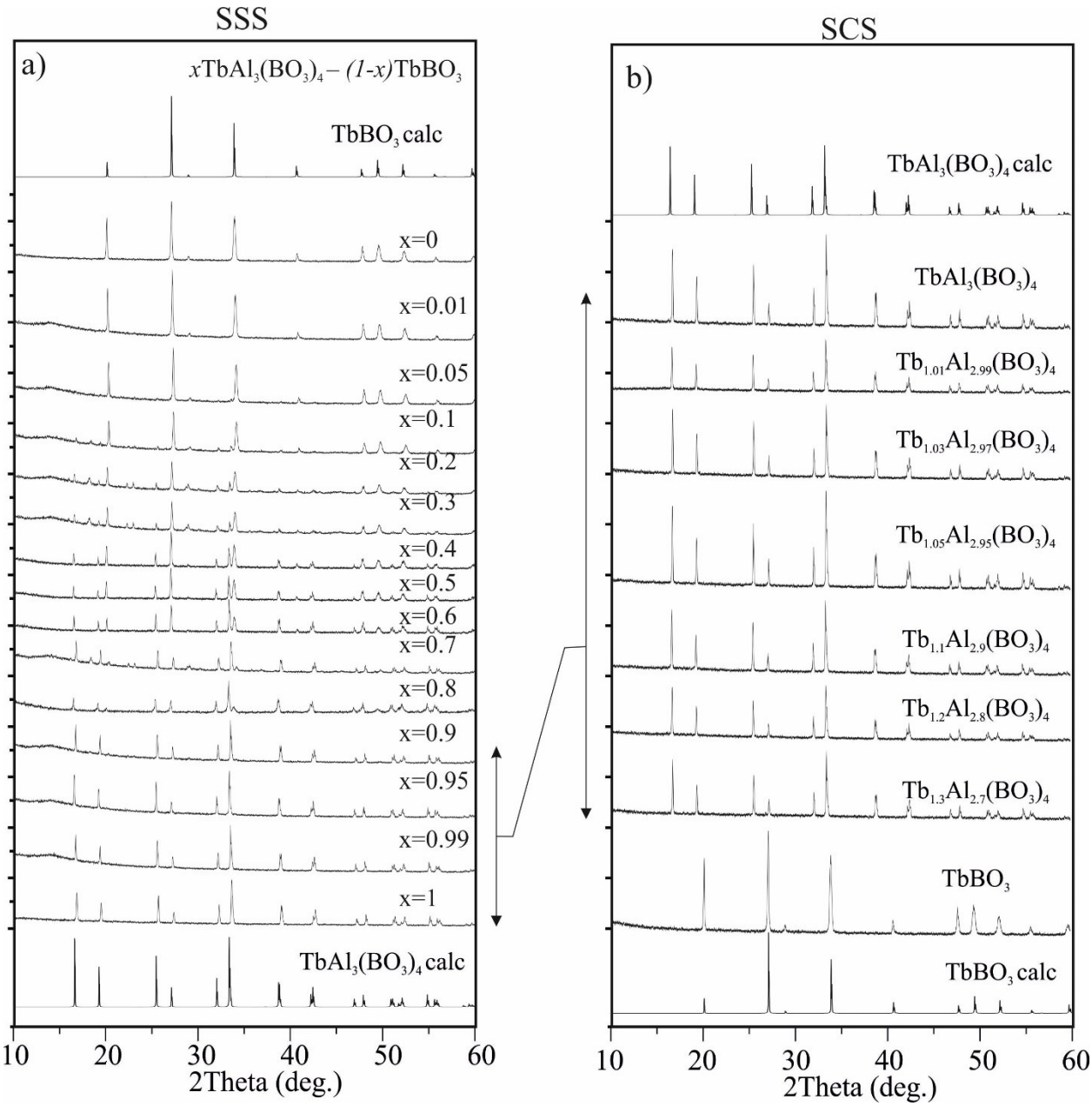

Figure S2. XRD patterns of xTbAl$_3$(BO$_3$)$_4$ – $(1-x)$TbBO$_3$ samples annealing at 1100 °C in Ar atmosphere.

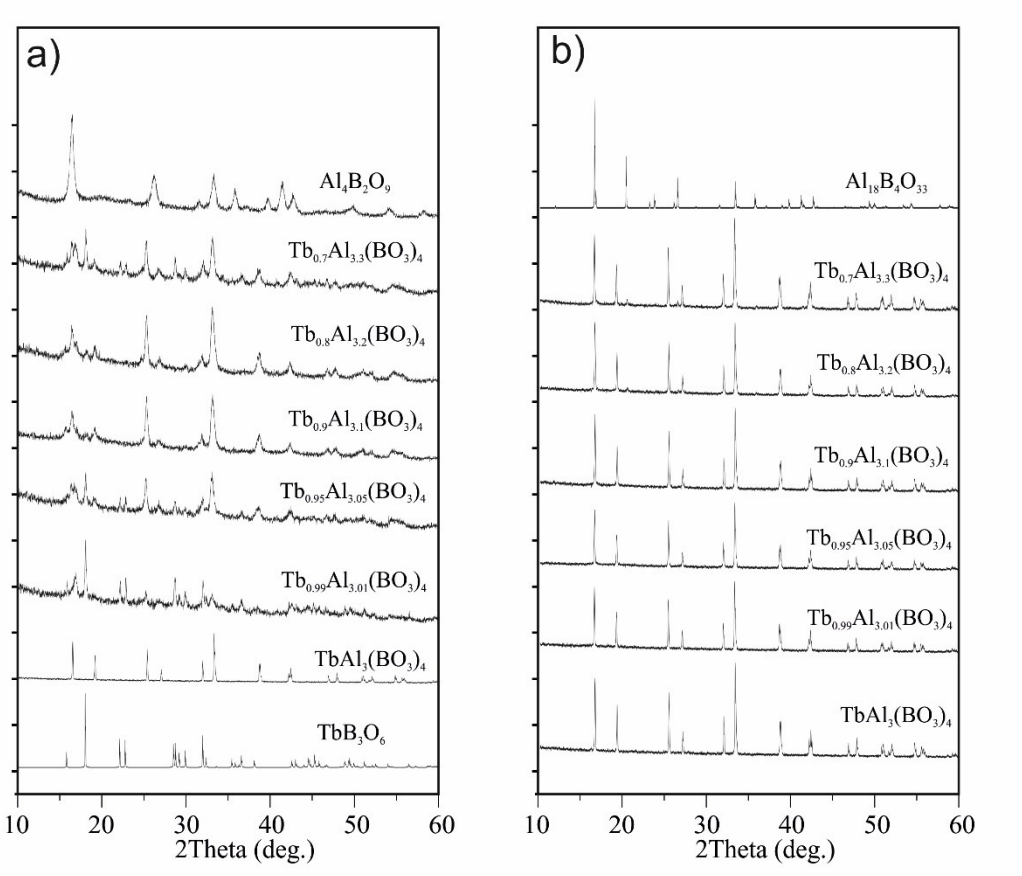

Figure S3 XRD patterns of $x\mathrm{TbAl_3(BO_3)_4}$ – $(1-x)\mathrm{Al_2O_3}$+$\mathrm{B_2O_3}$ samples annealing at a) 800 °C and b) 1200 °C in Ar atmosphere

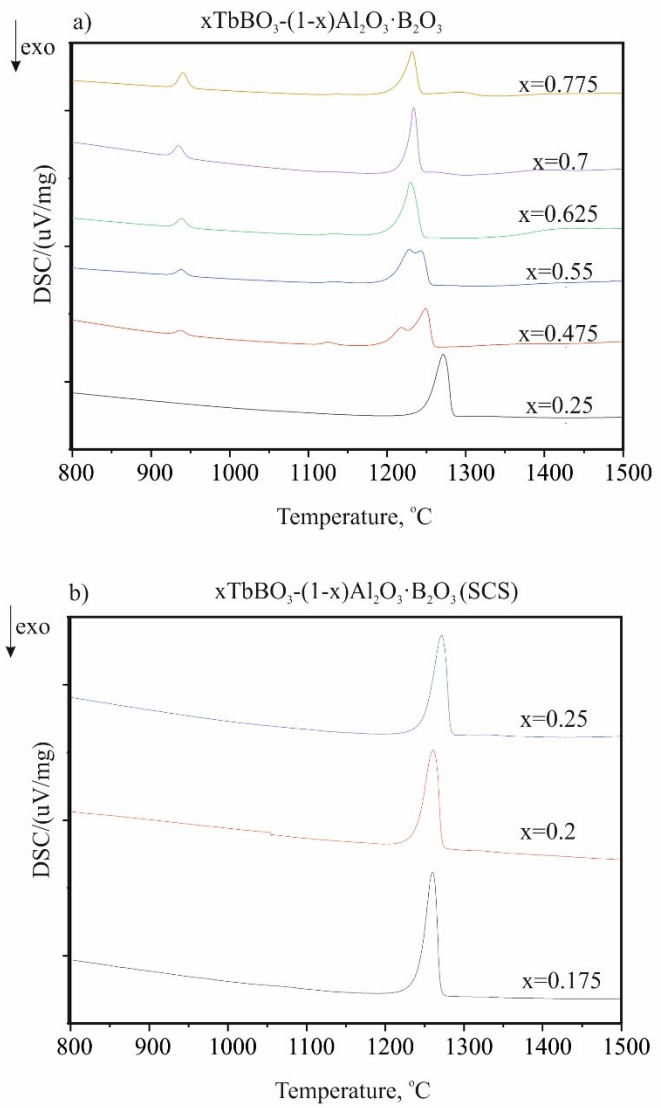

Figure S4. DSC curves of $x\mathrm{TbBO_3}$–$(1-x)\mathrm{Al_2O_3{\cdot}B_2O_3}$ samples syntheses by a) SSS (1100°C) and b) SCS (1200°C).

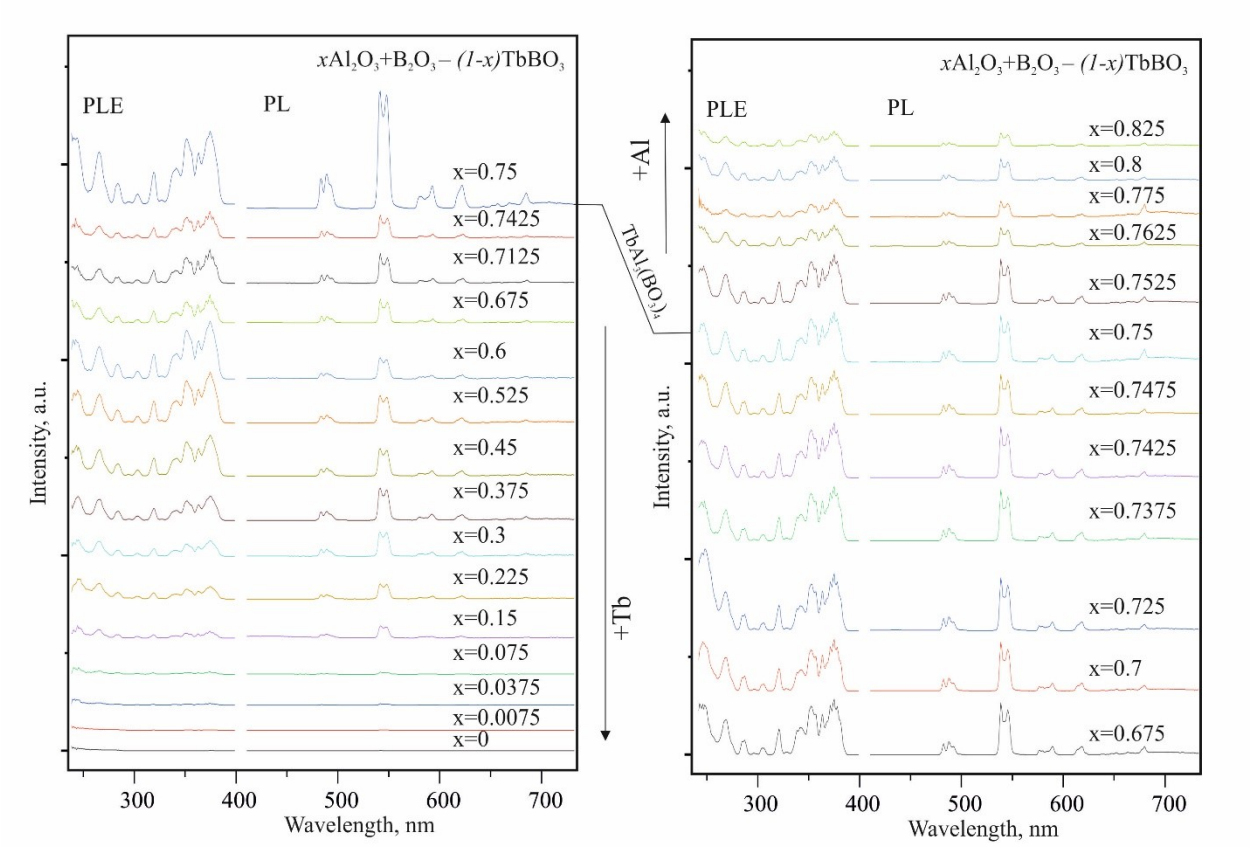

Figure S5 The excitation (PLE) and emission (PL) spectra of the a) $TbAl_3(BO3)_4$-$TbBO_3$ 1100°C_Ar and b) annealing at 1200 C after combusted method λ_{ex} = 375 nm, λ_{em} = 541 nm, T = 300 K

Table S2. Summary data about the powder XRD data-collection parameters, the Rietveld structure refinement of crystals from batch II (Figure 1).	
Empirical formula	$Tb_{1.12}Al_{2.88}(BO_3)_4$
Formula weight	490.89
Crystal system	trigonal
Space group	*R*32
a (Å)	9.2967(3)
b (Å)	9.2967(3)
c (Å)	7.2511(1)
α	90
β°	90
γ	120
Z	3
Volume ($Å^3$)	542.74(3)
Diffractometer	TD 3700(Tongda, China)
Radiation type	CuKa
Wavelength (A˚)	1.5418
Profile range (2teta)	10-120
Step size (12y)	0.02
Number of observation (N)	5499
Number of contributing reflections	113
Number of structure parameters (P1)	24
Number of profile parameters (P2)	10
RBragg (%)	8.44
Rp (%)	7.36
Rwp (%)	9.36
Rexp (%)	8.39
GOF	1.118

Table S3. The final atomic coordinates and equivalent isotropic displacement parameters in $Tb_{1.12}Al_{2.88}(BO_3)_4$.

Atom	x	y	z	occ	U_iso_or_equiv
Tb1	0	0	0	1	0.0226(9)
Tb2	0.5555(7)	0	0	0.040(6)	0.034(4)
Al3	0.5555(7)	0	0	0.960(6)	0.034(4)
B1	0	0	0,5	1	0.031(7)
B2	0.429(7)	0	0,5	1	0.031(7)
O1	0.1416(12)	0.1416(12)	0,5	1	0.016(2)
O2	0.4423(12)	0.1420(11)	0.519 (2)	1	0.016(2)
O3	0.578(3)	0	0,5	1	0.016(2)