Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2022

Supporting Information:

Presence of Irregular Oxidation State of Bi⁴⁺ and Single-Element White Emission in YAl₃(BO₃)₄: Bi

Shuai Yang, ^{‡,§} Yannan Dai, [‡] Jiwei Tan, [‡] Chungang Duan,^{‡, §} Qingbiao Zhao[‡]

[‡] Key Laboratory of Polar Materials and Devices (MOE), Department of Electronic Science, East China Normal University, Shanghai, 200241 China

^{\$} Collaborative Innovation Center of Extreme Optics, Shanxi University, Shanxi 030006, China

^{\$}Current affiliation: School of Materials Science and Engineering, Shanghai Jiao Tong University, Shanghai, 200240 China



Figure S1. The XRD patterns of YABO and YABO: Bi phosphors.



Figure S2. The shift of the XRD peaks for various YABO: Bi phosphors in the 2θ range of $31 \sim 35^{\circ}$.

	YABO	YABO:0.01Bi
Space group	$P6_3$	$P6_3$
a (Å)	9.28355	9.27495
b (Å)	9.28355	9.27495
c (Å)	7.22959	7.22388
V (Å ³)	539.601	538.0769
R _{wp}	9.90 %	6.660 %
R _p	7.60 %	5.184 %
R _{exp}	5.897 %	2.517 %
gof	1.68	1.17

Table S1. The lattice parameters and Rietveld refinement parameters for YABO andYABO:0.01Bi

Atom	Х	у	Z	occupancy
Y1	0	0	0	1.0
A11	0.55517	0	0	1.0
B1	0	0	0.5	1.0
B2	0.4317	0	0.5	1.0
01	0.84955	0	0.5	1.0
O2	0.58618	0	0.5	1.0
O3	0.44504	0.14799	0.52948	1.0

Table S2. Atomic coordinates of YABO obtained by Rietveld refinement

Atom	Х	У	Z	occupancy
Y	0	0	0	0.99
Bi	0	0	0	0.01
Al	0.55528	0	0	1.0
B1	0	0	0.5	1.0
B2	0.44322	0	0.5	1.0
01	0.85058	0	0.5	1.0
O2	0.59066	0	0.5	1.0
03	0.44843	0.14899	0.52435	1.0

Table S3. Atomic coordinates of YABO: 0.01Bi obtained by Rietveld refinement



Figure S3. The UV-Vis diffuse reflectance spectrum of YABO: Bi phosphors.