

Electronic Supplementary Material (ESI)

A New Lead-free Perovskite $\text{Rb}_7\text{Bi}_3\text{Cl}_{16}$ Nanocrystals with High Luminescence Properties and Excellent Moisture-Stability

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Table S1. Crystal data and structure refinement for Rb₇Bi₃Cl₁₆.

Compound	Rb ₇ Bi ₃ Cl ₁₆
Formula weight	1792.43
Wavelength (Å)	0.71073
Temperature (K)	298(2)
Crystal System	trigonal
Space Group	<i>P</i> -31c
<i>a</i> (Å)	7.5561(3)
<i>b</i> (Å)	7.5561(3)
<i>c</i> (Å)	34.3002(16)
α (°)	90
β (°)	90
γ (°)	120
Volume <i>V</i> /Å ³	1695.99(12)
<i>Z</i>	2
Density ρ_{cal} (g/cm ³)	3.510
Absorption coefficient μ (mm ⁻¹)	26.763
<i>F</i> (000)	1560
Theta range for data collection θ (°)	3.11 - 26.32
	$-8 \leq h \leq 9$
Limiting indices	$-9 \leq k \leq 9$
	$-42 \leq l \leq 42$
Reflections collected/unique	16424 / 1172
goodness of fit on <i>F</i> ²	1.065
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> > 2σ (<i>I</i>)] ^a	0.0432, 0.1053
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0469, 0.1081
Largest diff. peak and hole (e ⁺ •Å ⁻³)	1.847 and -1.824

$$^a R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|; wR_2 = [\Sigma w(F_o^2 - F_c^2)^2] / [\Sigma w(F_o^2)^2]^{1/2}$$

Table S2. A Summary about different octahedral distortion of Rb₇Bi₃Cl₁₆.

Octahedron	[Bi(1)Cl ₆] ³⁻	[Bi(2) ₂ Cl ₁₀] ⁴⁻
$\triangle d$	0	0.84
Distortion Degree	Ideal octahedron	Strong distortion

Table S3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Rb}_7\text{Bi}_3\text{Cl}_{16}$. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
Bi(1)	0	0	5000	42(1)
Bi(2)	3333	6667	1845(1)	35(1)
Cl(1)	3330(6)	2030(9)	4551(2)	109(2)
Cl(2)	6155(16)	8077(8)	2500	47(3)
Cl(3)	525(17)	5263(8)	2500	57(3)
Cl(4)	3493(12)	10321(11)	1851(2)	42(2)
Cl(5)	3491(12)	3152(11)	1844(2)	44(2)
Cl(6)	834(15)	5392(16)	1271(3)	63(2)
Cl(7)	6307(15)	8152(15)	1359(4)	71(3)
Rb(1)	0	0	2500	46(1)
Rb(2)	3333	6667	4648(1)	70(1)
Rb(3)	0	0	3781(1)	49(1)
Rb(4)	5755(5)	2871(5)	3846(1)	43(1)
Rb(5)	-2804(3)	2804(3)	2500	43(1)

Table S4 Semi-quantitative analysis results of XPS.

Element	BE [eV]	Atomic conc. [%]
Rb 3d	106.60	31.10
Bi 4f	156.40	15.04
Cl 2p	195.10	53.86

Table S5 Comparison of stability for the different Bi-based nanocrystals.

Sample (NCs)	$\text{Rb}_7\text{Bi}_3\text{Cl}_{16}$	$\text{Cs}_3\text{Bi}_2\text{Br}_9$	$\text{Cs}_2\text{AgBiBr}_6$	$\text{MA}_3\text{Bi}_2\text{Br}_9$
Thermal-stability	Stable below 400 °C	Stable below 496 °C	Stable below 430 °C	Stable below 200 °C
Moisture-stability	Maintain about 70% PL after one month	Maintain 90% PL after 8 hours	No report on NCs' moisture-stability	Completely decomposition in 8 hours
PLQY	28.43%	19.4%	0.7%	12%
Reference	This work	1	2, 3	1,4

References

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2. W. Pan, H. Wu, J. Luo, Z. Deng, C. Ge, C. Chen, X. Jiang, W. Yin, G. Niu, L. Zhu, L. Yin, Y. Zhou, Q. Xie, X. Ke, M. Sui and J. Tang, *Nature Photonics*, 2017, **11**, 726–732.
3. B. Yang, J. Chen, S. Yang, F. Hong, L. Sun, P. Han, T. Pullerits, W. Deng, and K. Han, *Angew. Chem. Int. Ed.*, 2018, **57**, 5359–5363.
4. M. Leng, Z. Chen, Y. Yang, Z. Li, K. Zeng, K. Li, G. Niu, Y. He, Q. Zhou, J. Tang, *Angew. Chem. Int. Ed.*, 2016, **55**, 15012–15016.

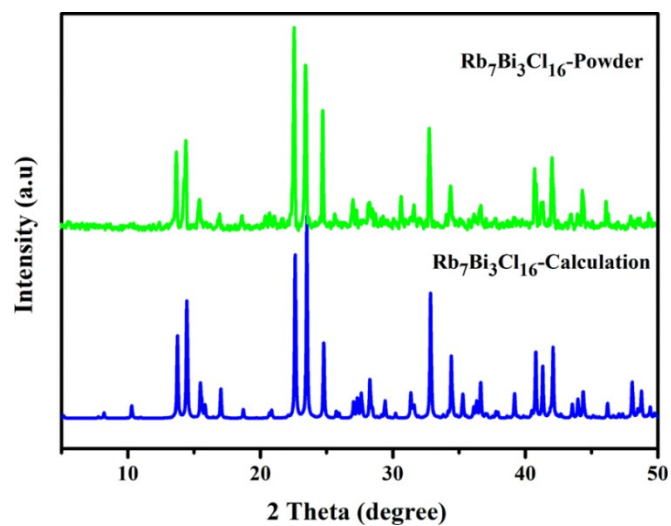


Figure S1. Experimental and simulated powder X-ray diffraction patterns of $\text{Rb}_7\text{Bi}_3\text{Cl}_{16}$.

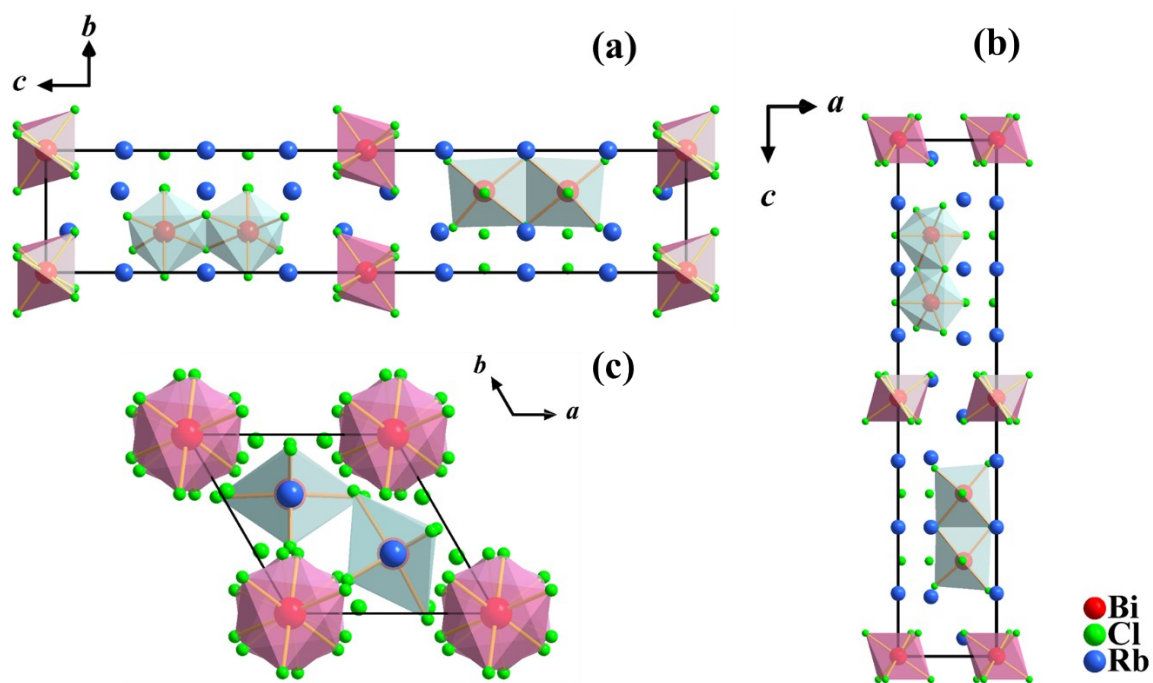


Figure S2. Unit cell of $\text{Rb}_7\text{Bi}_3\text{Cl}_{16}$ (a) along the a -axis, (b) along the b -axis and (c) along the c -axis.

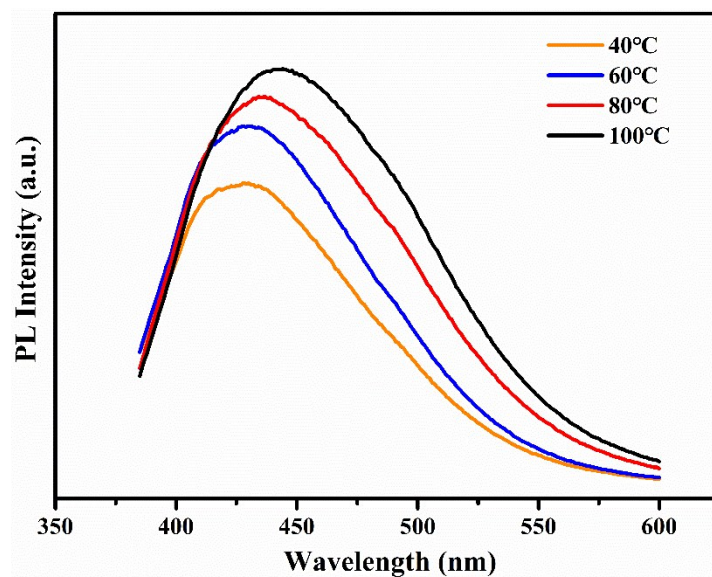


Figure S3. The PL of $\text{Rb}_7\text{Bi}_3\text{Cl}_{16}$ NCs prepared under different reaction temperature.

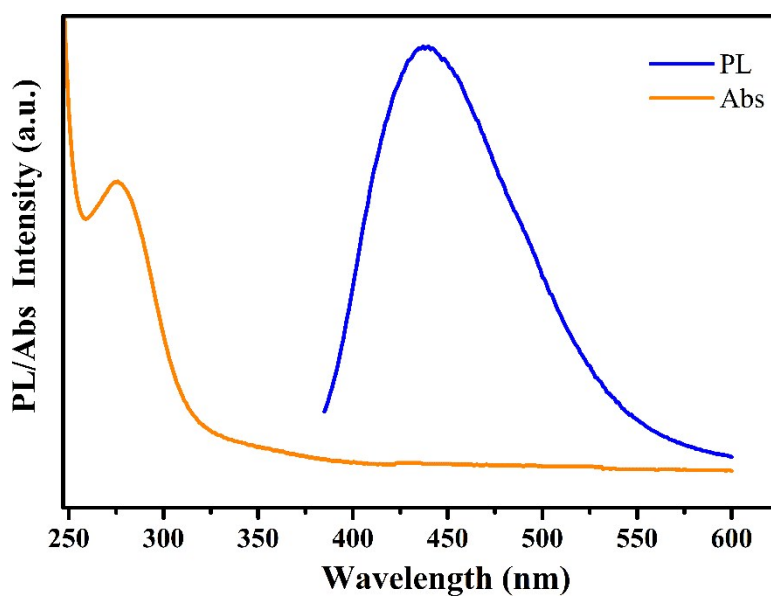


Figure S4. The Absorption and PL spectra of $\text{Rb}_7\text{Bi}_3\text{Cl}_{16}$ NCs.

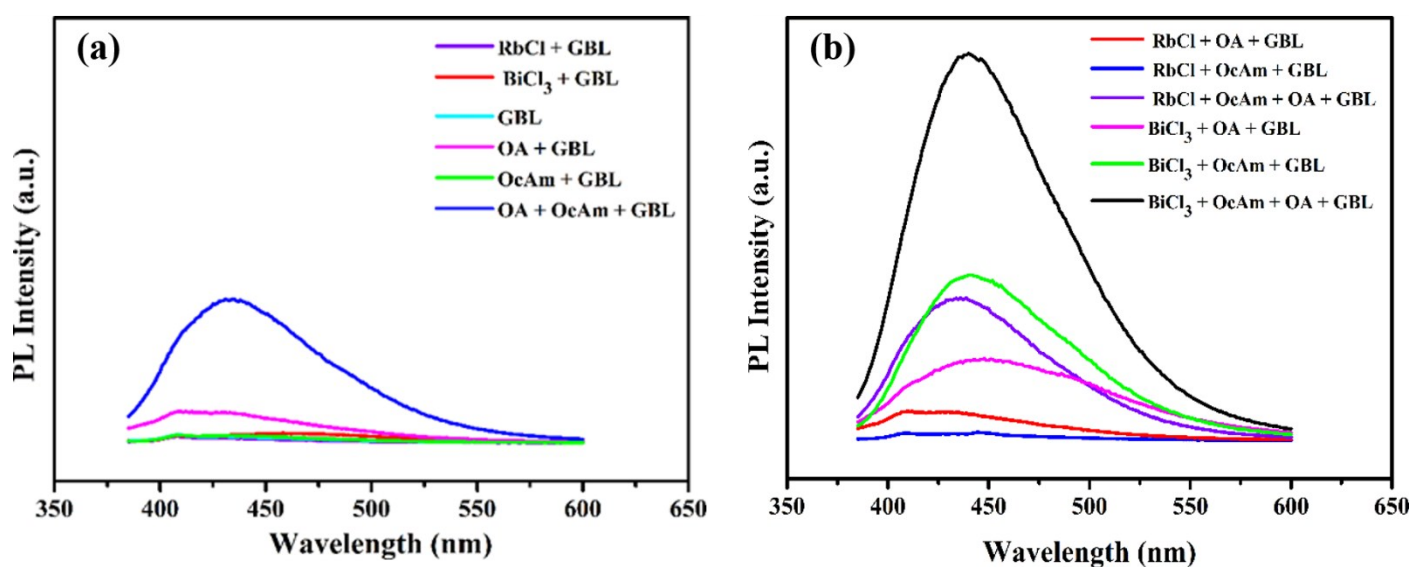


Figure S5. PL spectra of different reaction substrates.

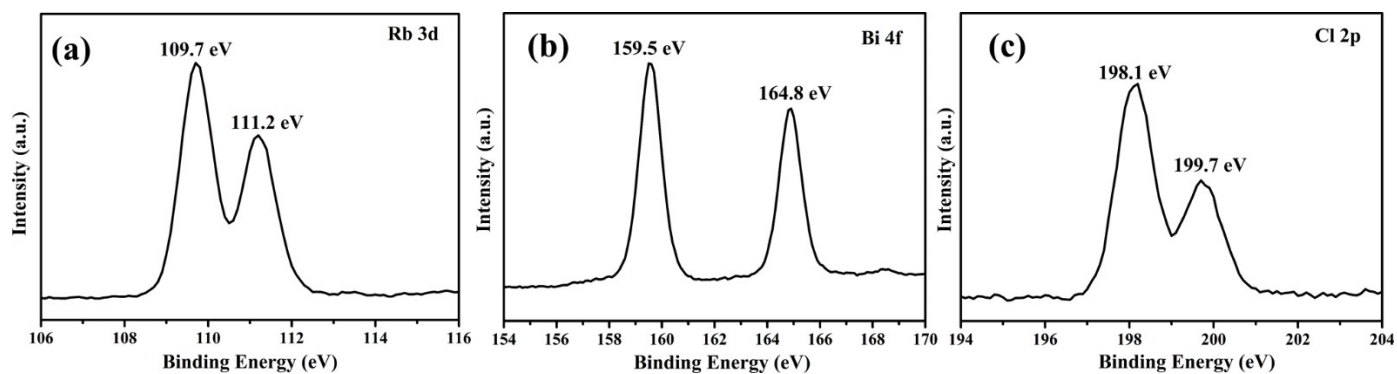


Figure S6. XPS spectra of $\text{Rb}_7\text{Bi}_3\text{Cl}_{16}$ NCs powder.

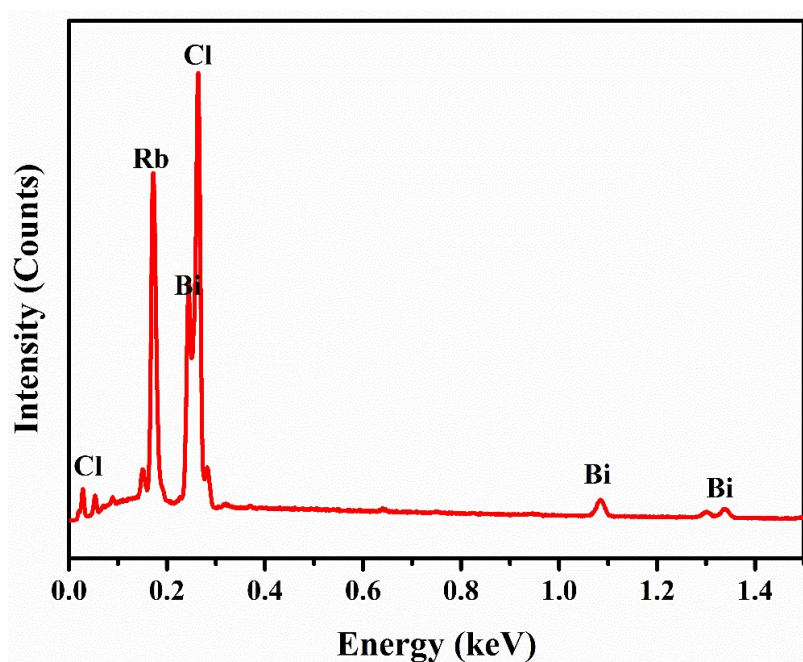


Figure S7. EDS of $\text{Rb}_7\text{Bi}_3\text{Cl}_{16}$ NCs powder.

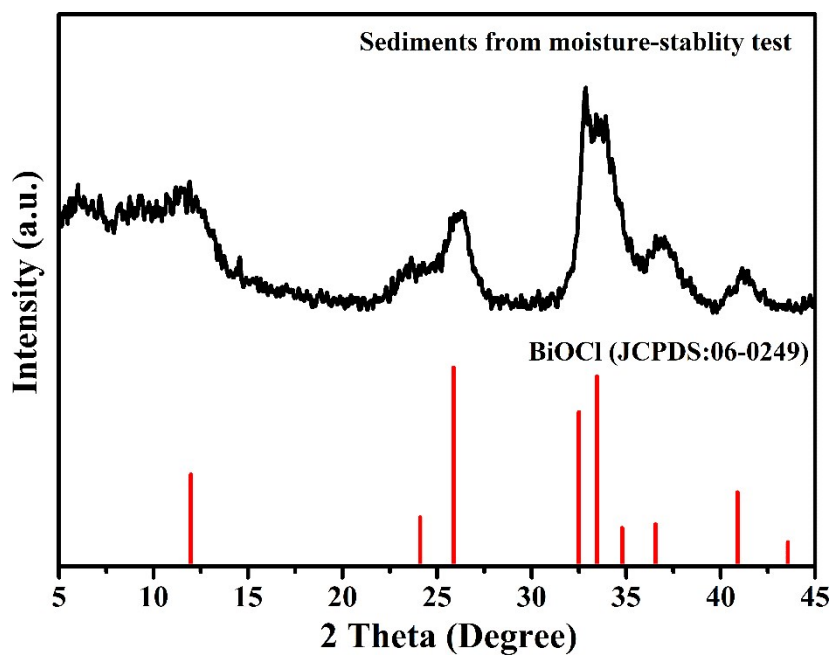


Figure S8. Powder XRD of the deposits obtained from moisture-stability test after 4 hours.