

Supporting information

The effect of n-Butanol on regulating the solubility-temperature characteristics for the Growth of High-Quality CsPbBr₃ Single Crystals

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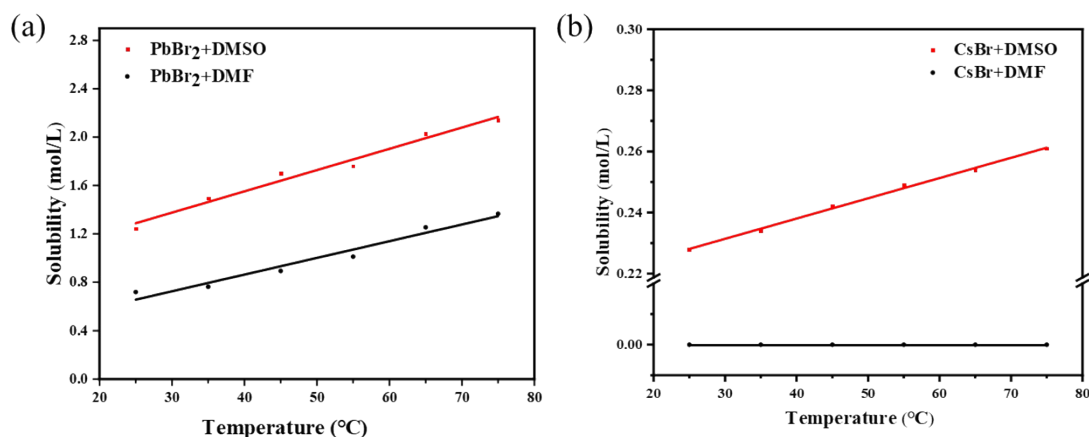


Figure S1. (a) Solubility curves of PbBr₂ in DMSO and DMF. (b) Solubility curves of CsBr in DMSO and DMF.

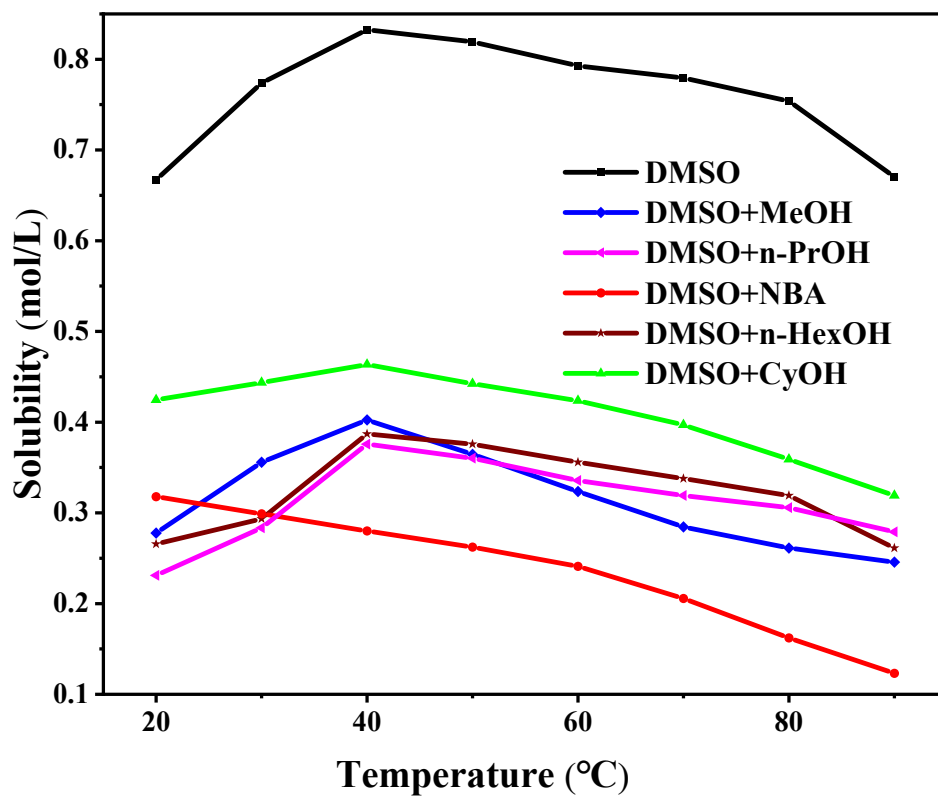


Figure S2. Solubility curves of CsPbBr₃ in DMSO and DMSO with different alcohols added.

Table S1 Summary of the growth of CsPbBr₃ single crystals.

Reference	Solvent	Additives	Growth method	Growth temperature (°C)	XRC (°)	τ or $\mu\tau$ (ns or cm ² /V)
[1]	DMSO	none	LTC ^a	27-30	none	none
[2]	DMSO	none	ITC ^b	110	none	$\tau_2=17.03$
[3]	DMSO	none	ITC ^b	140	0.043	none
[4]	DMSO	Choline Bromide	ITC ^b	80-85	none	$\mu\tau_e=1.80 \times 10^{-3}$
[5]	DMSO	TMAB	ITC ^b	60-85	none	$\tau_{ave}=88$
[6]	DMSO	Bromoacetic acid	ITC ^b	105	0.07	$\tau=80$
[7]	DMSO	none	ITC ^b	85	none	$\mu\tau_h=9.01 \times 10^{-4}$
[8]	DMSO/DMF	Acetonitrile	ITC ^b	45-60	0.035	$\mu\tau=2.57 \times 10^{-4}$
[9]	DMSO/DMF/CyOH	none	ITC ^b	90-110	none	$\mu\tau=2 \times 10^{-4}$
[10]	DMSO/DMF/CyOH	none	ITC ^b	49.5	none	$\tau_1=2.9;$ $\tau_2=25.1$
[11]	DMSO/DMF/CyOH	none	ITC ^b	50-90	none	none
[12]	DMSO/DMF/CyOH	none	ITC ^b	40-80	none	$\mu\tau=2.8 \times 10^{-4}$
[13]	DMSO/DMF/CyOH	Choline Bromide	ITC ^b	below 85	0.082	$\tau_1=0.70$ $\tau_2=6.51$
[14]	DMSO/DMF/CyOH	4-bromobutyric acid	ITC ^b	60-85	0.025	$\mu\tau_h=0.57 \times 10^{-4}$
This work	DMSO	n-butanol	ITC ^b	50-85	0.035	$\mu\tau_h=0.67 \times 10^{-4}$

a LTC: Low-temperature crystallization; b ITC: Inverse temperature crystallization

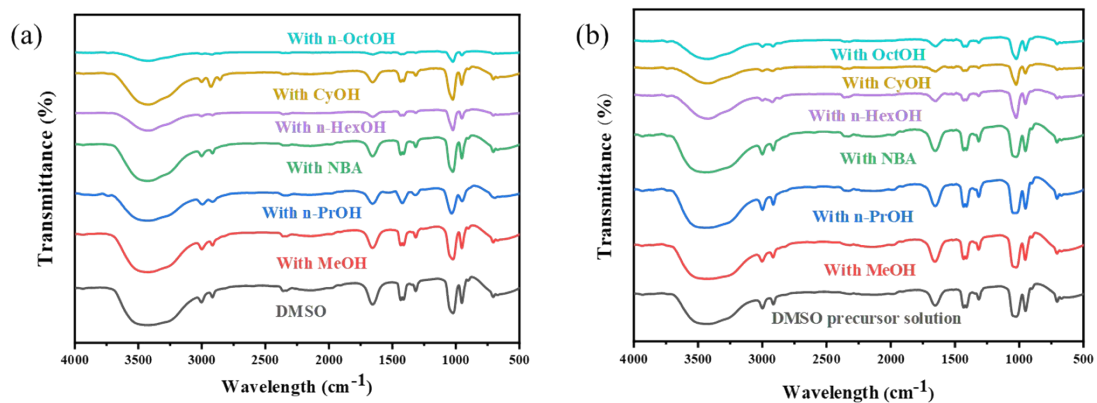


Figure S3. (a) FTIR spectra of different alcohols mixed in DMSO. (b) FTIR spectra of different alcohols mixed in CsPbBr₃ precursor solution.

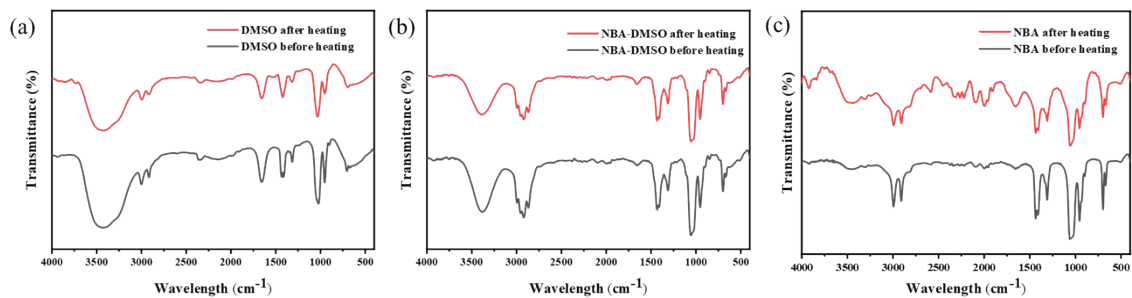

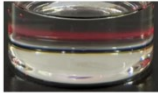





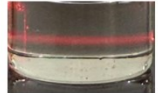









Figure S4. FTIR spectra of different solvents before and after thermal treatment: (a) pure DMSO, (b) NBA in DMSO, and (c) pure NBA.

Table S2 Summary of Tyndall effect in different precursors containing different alcohols at 30°C~70°C.

Temperature	30°C	40°C	50°C	60°C	70°C
DMSO					
DMSO+DMF +CyOH					
DMSO+NBA					

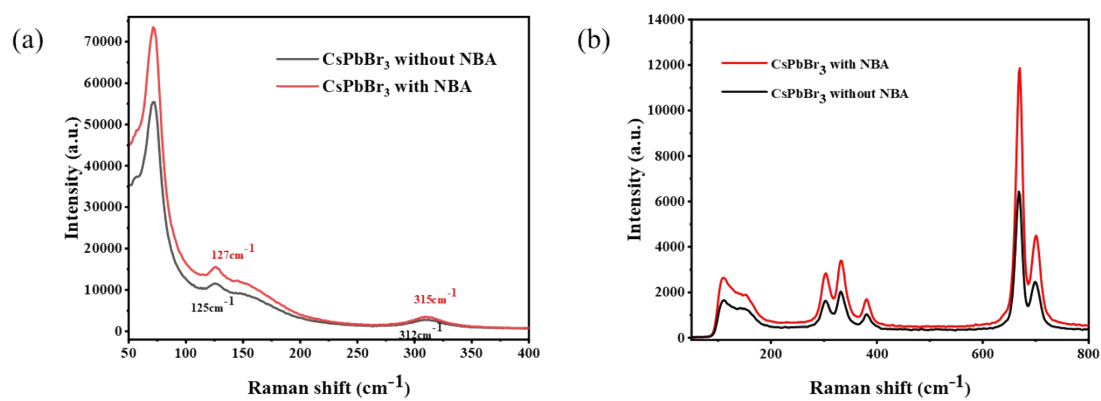


Figure S5. (a) Raman spectra of CsPbBr₃ powders synthesized with and without NBA additive. (b) Raman spectra of CsPbBr₃ solution grown with or without NBA additive.

Table S3 Key solvent parameters of different alcohols.

Solvent	DN (kcal/mol)	σ (Å)	ϵ_r (25°C)	μ (D)
Methanol	19	3.6	32.7	1.7
n-Propanol	21.1	4.7	20.5	1.58
n-Butanol	19.5	5.0	17.5	1.66
n-Hexanol	17.4	5.4	13.0	1.60
Cyclohexanol	~20	5.8	15.9	1.85
DMSO	29.8	4.4	46.7	3.96

The data comes from [15-18].

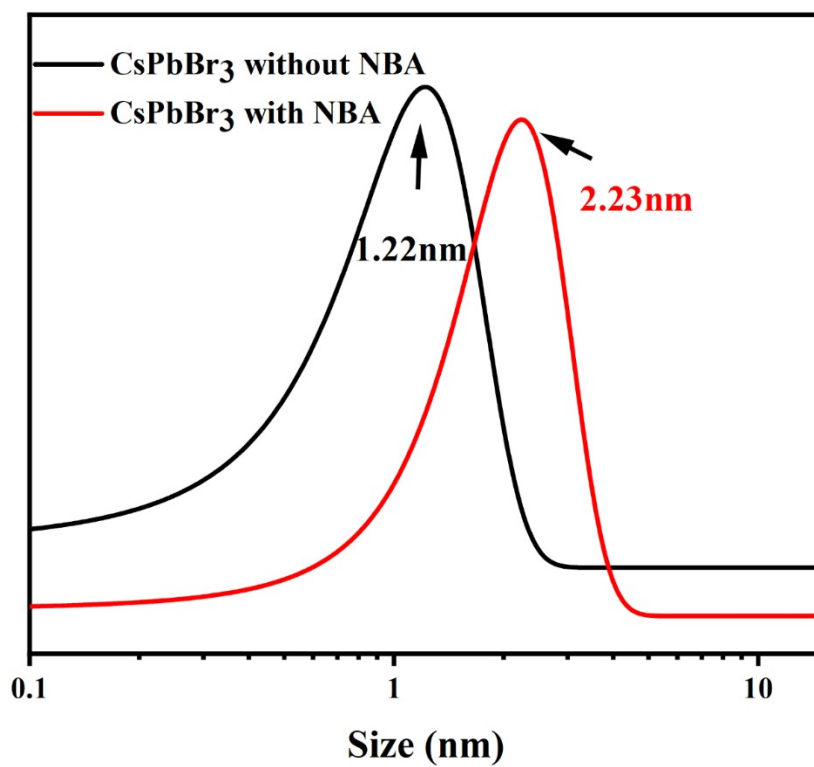


Figure S6. Particle size diagram of CsPbBr₃ precursor solution with and without NBA

addition.

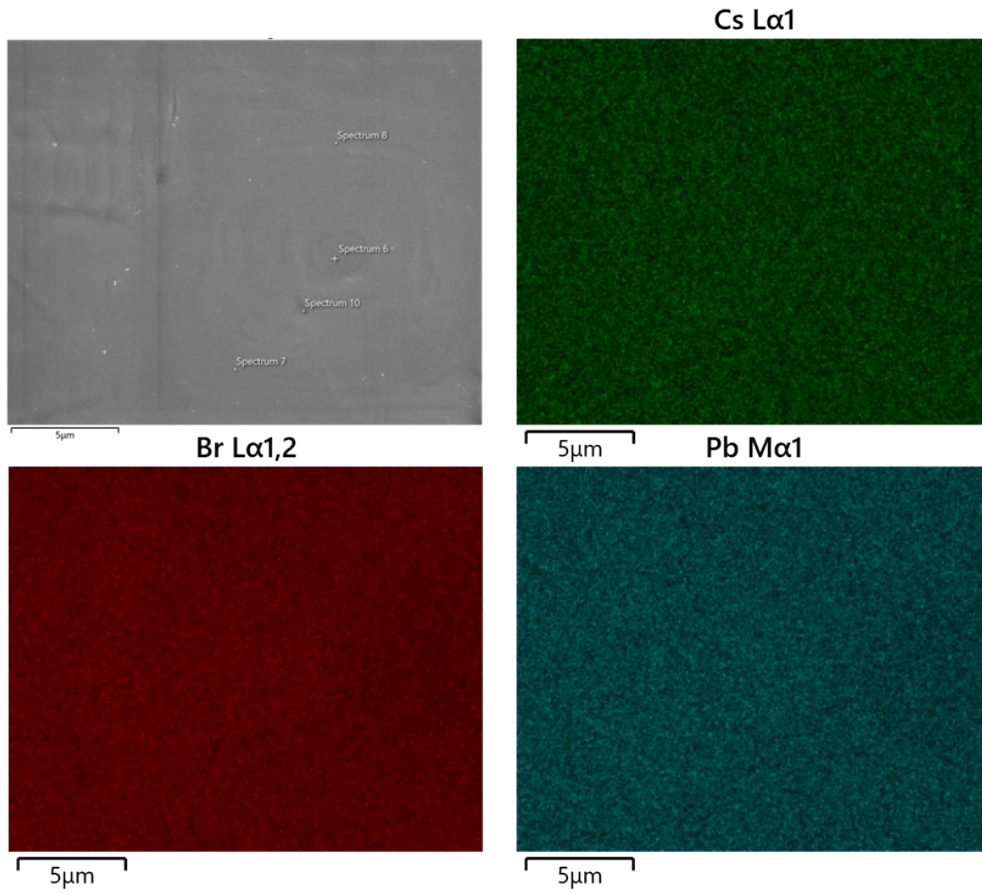


Figure S7. SEM and corresponding EDS elemental mapping images of CsPbBr₃ crystal surface.

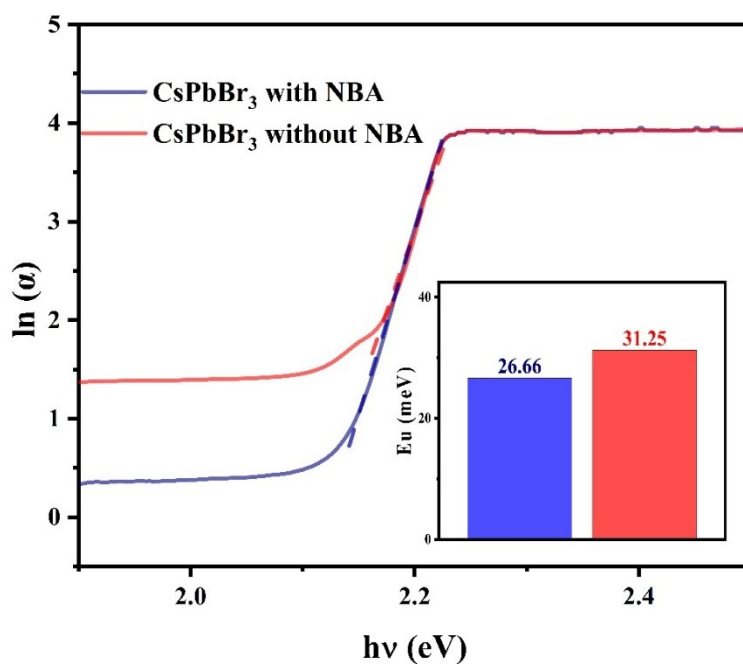


Figure S8. Urbach energy analysis of the CsPbBr₃ single crystal grown.

Table S4 Quantitative elemental analysis of CsPbBr₃ crystals via EDS point-scan mode.

Element	Spectrum 6		Spectrum 7		Spectrum 9		Spectrum 10		Map Sum Spectrum	
	at.%	ratio	at.%	ratio	at.%	ratio	at.%	ratio	at.%	ratio
Cs	21.64	1	21.48	1	21.63	1	22.05	1	21.30	1
Pb	20.96	0.97	20.78	0.97	20.86	0.96	20.61	0.94	20.60	0.97
Br	57.39	2.65	57.73	2.69	57.51	2.66	57.34	2.60	58.10	2.73
Total	100	CsPbBr ₃	100	CsPbBr ₃	100	CsPbBr ₃	100	CsPbBr ₃	100	CsPbBr ₃

References

1. P. Sujith, M. Pratheek, S. R. Parne and P. Predeep, *J. Electron. Mater.*, 2023, **52**, 718-729.
2. L. Gao, J.-L. Sun, Q. Li and Q. Yan, *ACS Appl. Mater. Interfaces*, 2022, **14**, 37904-37915.
3. M. Chen, Y. Yuan, Y. Liu, D. Cao and C. Xu, *RSC Adv.*, 2022, **12**, 14838-14843.
4. Y. Feng, L. Pan, H. Wei, Y. Liu, Z. Ni, J. Zhao, P. N. Rudd, L. R. Cao and J. Huang, *J. Mater. Chem. C*, 2020, **8**, 11360-11368.
5. L. Pan, Z. Liu, C. Welton, V. V. Klepov, J. A. Peters, M. C. De Siena, A. Benadia, I. Pandey, A. Miceli, D. Chung, G. N. M. Reddy, B. W. Wessels and M. G. Kanatzidis, *Adv. Mater.*, 2023, **35**, 2211840.
6. Z. Xue, Y. Wei, H. Li, J. Peng, F. Yao, Y. Liu, S. Wang, Q. Zhou, Q. Lin and Z. Wang, *Small*, 2023, **19**, 2207588.
7. H. Qin, N. Shen, B. Xiao, X. He, Y. Wang, Q. Sun, S. Wei, X. Ouyang, B. Zhou, Z. Wu, Q. Min, R. Ren, N. Ding, W. Chen, X. Wang, Z. Chai, X. Ouyang and Y. He, *Adv. Funct. Mater.*, 2025, **35**, e09390.
8. K. Mou, X. Feng, F. Tang, W. Wang, X. Tang, Y. Liu, B. Zeng, S. Bao, M. Cui, J. Hu, H. Gou, Y. Zhu, J. Liu and R. Xu, *Journal of Materials Chemistry C*, 2025, **13**: 9154.
9. D. N. Dirin, I. Cherniukh, S. Yakunin, Y. Shynkarenko and M. V. Kovalenko, *Chem. Mater.*, 2016, **28**, 8470-8474.
10. H. Zhang, F. Wang, Y. Lu, Q. Sun, Y. Xu, B. Zhang, W. Jie and M. G. Kanatzidis, *J. Mater. Chem. C*, 2020, **8**, 1248-1256.
11. Y. Cheng, M. Zhu, F. Wang, R. Bai, J. Yao, W. Jie and Y. Xu, *J. Mater. Chem. A*, 2021, **9**, 27718-27726.
12. F. Wang, R. Bai, Q. Sun, X. Liu, Y. Cheng, S. Xi, B. Zhang, M. Zhu, S. Jiang, W. Jie and Y. Xu, *Chem. Mater.*, 2022, **34**, 3993-4000.
13. P. Cheng, Z. Liu, R. Kang, J. Zhou, X. Wang, J. Zhao and Z. Zuo, *ACS Omega*, 2023, **8**, 26351-26358.
14. Y. Liu, M. Cui, X. Feng, W. Wang, X. Tang, S. Bao, K. Mou, B. Zeng, F. Tang, J. Hu, H. Gou, J. Liu, Y. Zhu and R. Xu, *ACS Photonics*, 2025, **12(4)**: 2044-2052.
15. A. S. Tutantsev, N. N. Udalova, S. A. Fateev, A. A. Petrov, W. Chengyuan, E. G. Maksimov, E. A. Goodilin and A. B. Tarasov, *J. Phys. Chem. C*, 2020, **124**, 11117-11123.
16. C. M. Hansen, *Hansen Solubility Parameters: A User's Handbook*, 2nd ed., CRC Press, Boca Raton, 2007.
17. D. R. Lide, *CRC Handbook of Chemistry and Physics*, 103rd ed., CRC Press, Boca Raton, 2022-2023.
18. A. A. Petrov, A. A. Ordinartsev, S. A. Fateev, E. A. Goodilin and A. B. Tarasov, *Molecules*, 2021, **26(24)**, 7541.