

Electronic Supplementary Information (ESI) for:

Second-harmonic generation (SHG) and photoluminescence properties of
noncentrosymmetric (NCS) layered perovskite solid-solutions, $\text{CsBi}_{1-x}\text{Eu}_x\text{Nb}_2\text{O}_7$
($x = 0, 0.1, \text{ and } 0.2$)

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S1. Final Rietveld plot of $\text{CsBiNb}_2\text{O}_7$

S2. Final Rietveld plot of $\text{CsBi}_{0.9}\text{Eu}_{0.1}\text{Nb}_2\text{O}_7$

S3. Final Rietveld plot of $\text{CsBi}_{0.8}\text{Eu}_{0.2}\text{Nb}_2\text{O}_7$

S4. Atomic Coordinates, Displacement Parameters, and Occupancies for $\text{CsBiNb}_2\text{O}_7$

S5. Atomic Coordinates, Displacement Parameters, and Occupancies for $\text{CsBi}_{0.9}\text{Eu}_{0.1}\text{Nb}_2\text{O}_7$

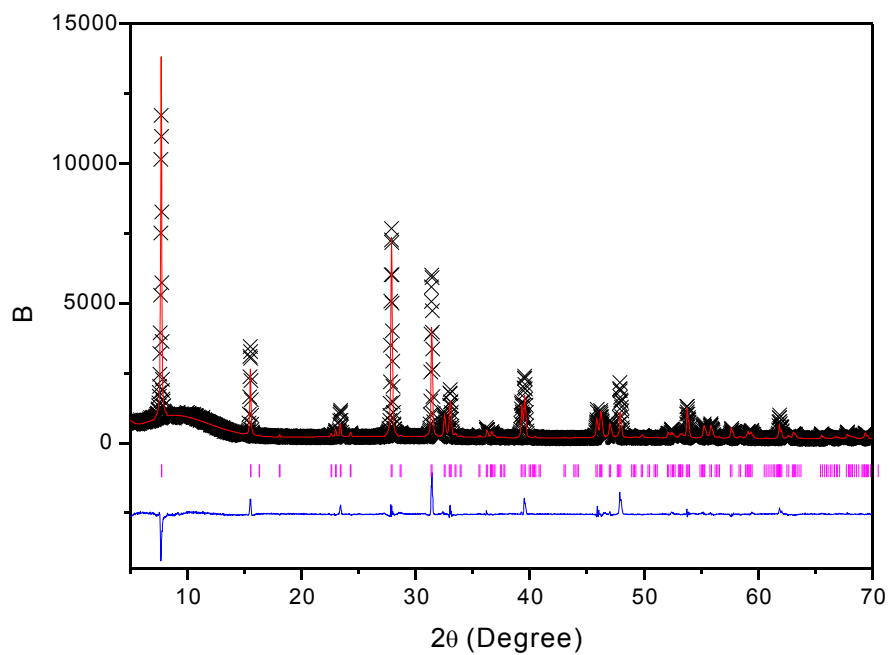
S6. Atomic Coordinates, Displacement Parameters, and Occupancies for $\text{CsBi}_{0.8}\text{Eu}_{0.2}\text{Nb}_2\text{O}_7$

S7. IR spectra for $\text{CsBi}_{1-x}\text{Eu}_x\text{Nb}_2\text{O}_7$ ($x = 0, 0.1, 0.2$) solid solutions

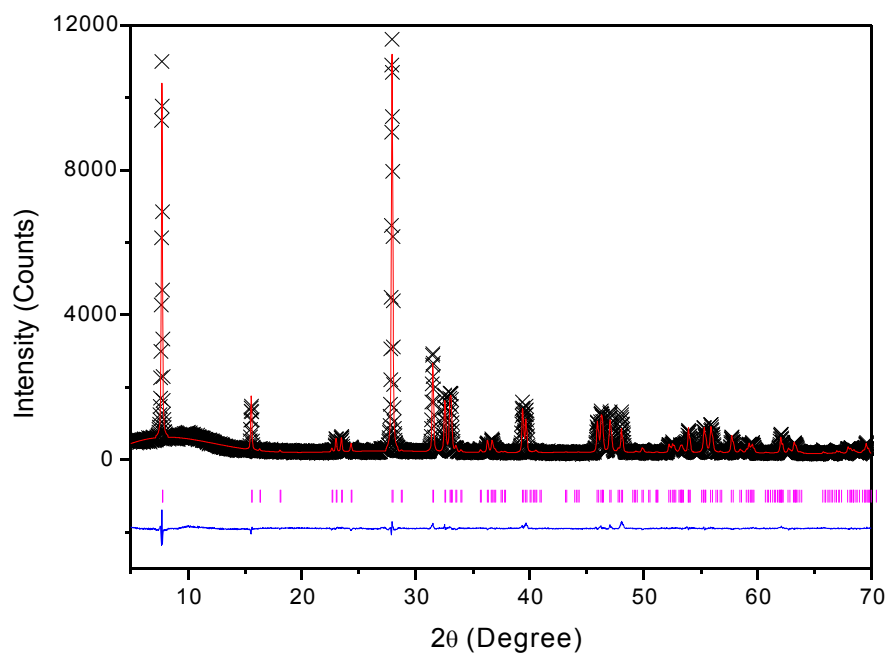
S8. UV-Vis diffuse reflectance spectra for $\text{CsBi}_{1-x}\text{Eu}_x\text{Nb}_2\text{O}_7$ ($x = 0, 0.1, 0.2$) solid solutions

S9. EDX spectra for $\text{CsBi}_{1-x}\text{Eu}_x\text{Nb}_2\text{O}_7$ ($x = 0, 0.1, 0.2$) solid solutions

S1. Final Rietveld plot of $\text{CsBiNb}_2\text{O}_7$

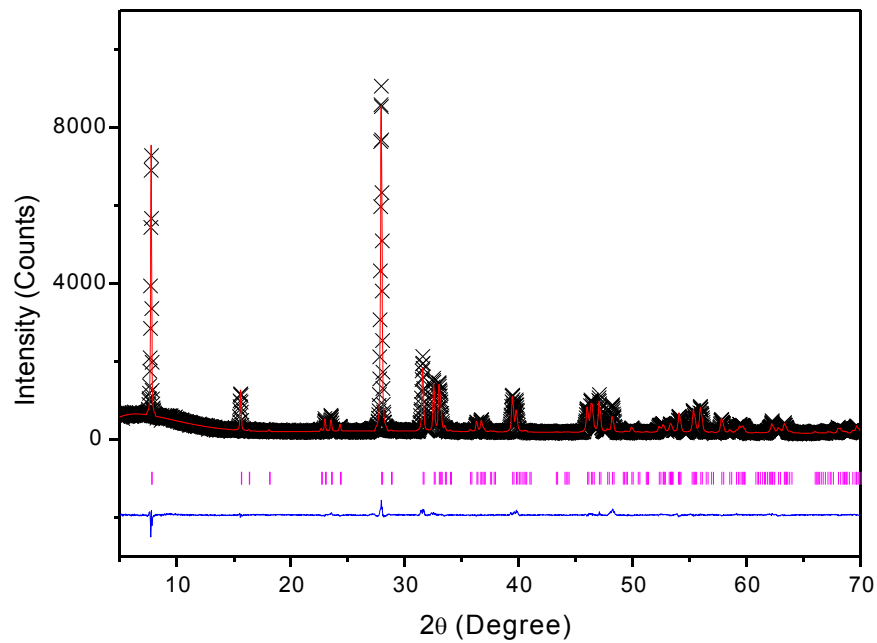


S2. Final Rietveld plot of $\text{CsBi}_{0.9}\text{Eu}_{0.1}\text{Nb}_2\text{O}_7$



The calculated pattern (red solid line) is compared with observed data (\times). The locations of reflections are indicated by the magenta vertical bars. The difference between the observed and calculated profiles is shown at the bottom (blue solid line).

S3. Final Rietveld plot of $\text{CsBi}_{0.8}\text{Eu}_{0.2}\text{Nb}_2\text{O}_7$



The calculated pattern (red solid line) is compared with observed data (×). The locations of reflections are indicated by the magenta vertical bars. The difference between the observed and calculated profiles is shown at the bottom (blue solid line).

S4. Atomic Coordinates, Displacement Parameters, and Occupancies for CsBiNb₂O₇

<i>Atom</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{iso}</i>	<i>Occupancy</i>
Cs(1)	0.755(5)	0.743(3)	0.5	0.018(2)	1.0
Bi(1)	0.8036(12)	0.7210(16)	0.0	0.009(2)	1.0
Nb(1)	0.2444(16)	0.757(3)	0.2101(3)	0.010(2)	1.0
O(1)	0.720(3)	0.339(16)	0.0	0.015(2) ^a	1.0
O(2)	0.240(3)	0.778(16)	0.3798(19)	0.015(2) ^a	1.0
O(3)	0.019(3)	0.071(14)	0.180(2)	0.015(2) ^a	1.0
O(4)	0.430(3)	0.434(13)	0.192(2)	0.015(2) ^a	1.0

^aDisplacement parameters constrained to be equal.

S5. Atomic Coordinates, Displacement Parameters, and Occupancies for CsBi_{0.9}Eu_{0.1}Nb₂O₇

<i>Atom</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{iso}</i>	<i>Occupancy</i>
Cs(1)	0.7549(13)	0.7403(16)	0.5	0.0318(15)	1.0
Bi(1)/Eu(1)	0.8008(9)	0.7240(9)	0.0	0.0223(9)	0.9/0.1 ^a
Nb(1)	0.2454(11)	0.7548(15)	0.2082(2)	0.0125(12)	1.0
O(1)	0.721(8)	0.298(10)	0.0	0.015(2) ^b	1.0
O(2)	0.242(6)	0.774(9)	0.3603(13)	0.015(2) ^b	1.0
O(3)	0.019(11)	0.039(8)	0.1676(15)	0.015(2) ^b	1.0
O(4)	0.419(7)	0.452(7)	0.1907(15)	0.015(2) ^b	1.0

^aStatistically disordered with 90% Bi³⁺ and 10% Eu³⁺. Atomic coordinates constrained to be equal.

^bDisplacement parameters constrained to be equal.

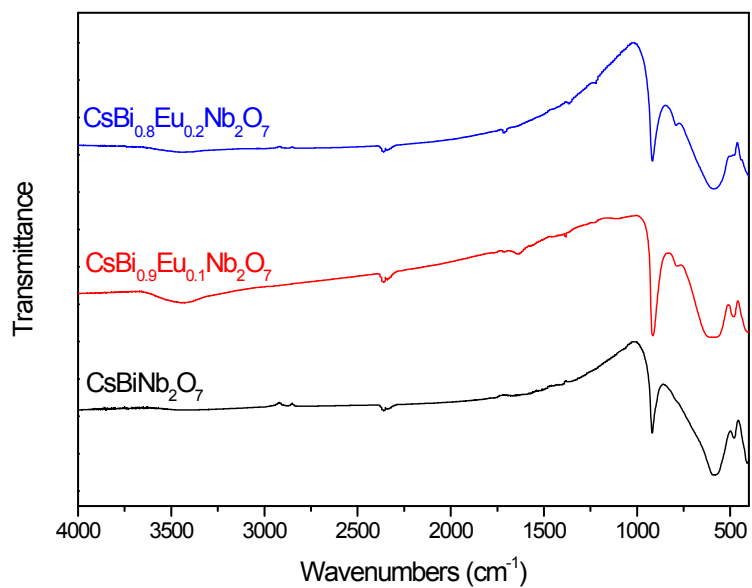
S6. Atomic Coordinates, Displacement Parameters, and Occupancies for CsBi_{0.8}Eu_{0.2}Nb₂O₇

<i>Atom</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{iso}</i>	<i>Occupancy</i>
Cs(1)	0.7577(13)	0.7407(17)	0.5	0.0109(15)	1.0
Bi(1)/Eu(1)	0.8048(10)	0.7244(10)	0.0	0.0084(9)	0.8/0.2 ^a
Nb(1)	0.2492(13)	0.7551(17)	0.2083(3)	0.0125(14)	1.0 ^a
O(1)	0.710(9)	0.313(10)	0.0	0.015(2) ^b	1.0
O(2)	0.242(7)	0.777(9)	0.3647(15)	0.015(2) ^b	1.0
O(3)	0.024(13)	0.033(10)	0.1693(17)	0.015(2) ^b	1.0
O(4)	0.409(7)	0.462(7)	0.1917(18)	0.015(2) ^b	1.0

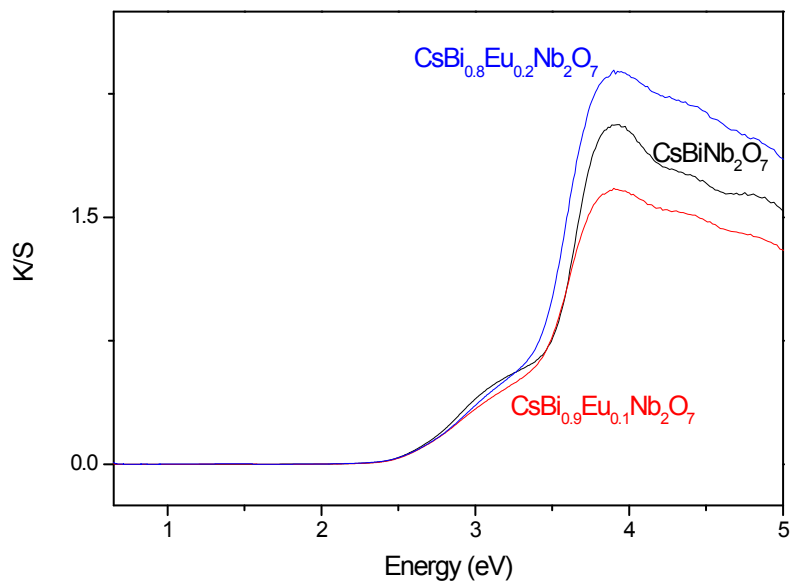
^aStatistically disordered with 80% Bi³⁺ and 20% Eu³⁺. Atomic coordinates constrained to be equal.

^bDisplacement parameters constrained to be equal.

S7. IR spectra for $\text{CsBi}_{1-x}\text{Eu}_x\text{Nb}_2\text{O}_7$ ($x = 0, 0.1, 0.2$) solid solutions

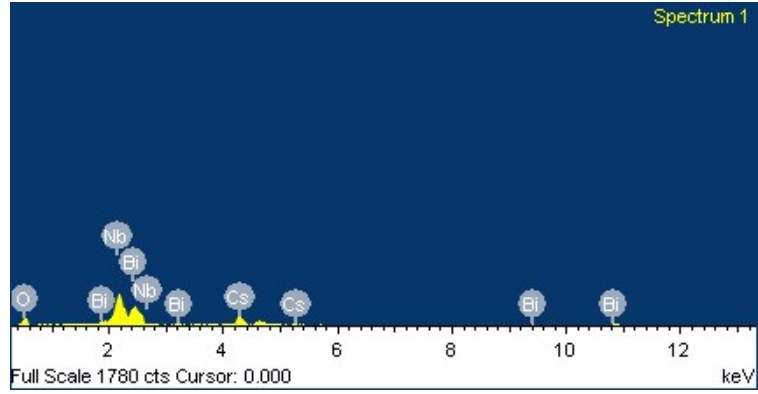


S8. UV-Vis diffuse reflectance spectra for $\text{CsBi}_{1-x}\text{Eu}_x\text{Nb}_2\text{O}_7$ ($x = 0, 0.1, 0.2$) solid solutions

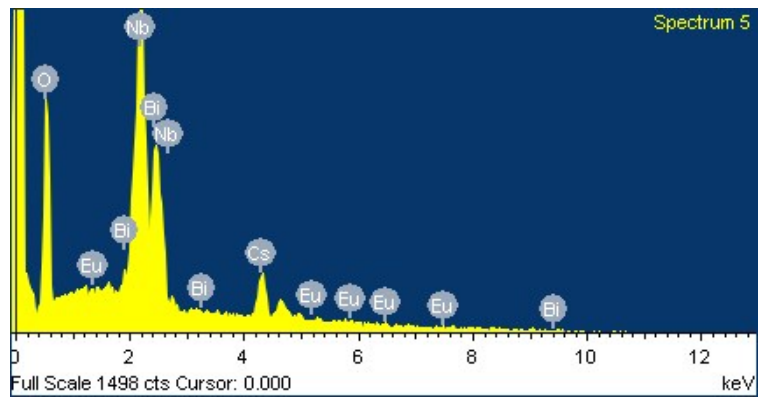


S9. EDX spectra for $\text{CsBi}_{1-x}\text{Eu}_x\text{Nb}_2\text{O}_7$ ($x = 0, 0.1, 0.2$) solid solutions

(1) $\text{CsBiNb}_2\text{O}_7$



(2) $\text{CsBi}_{0.9}\text{Eu}_{0.1}\text{Nb}_2\text{O}_7$



(3) $\text{CsBi}_{0.8}\text{Eu}_{0.2}\text{Nb}_2\text{O}_7$

