

Supporting Information

Non-Hygrosopic, Self-Absorption Free, and Efficient 1D CsCu₂I₃ Perovskite

Single Crystal for Radiation Detection

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EXPERIMENTAL METHODS

Crystal growth

The 99.99% purity CsI powders from Griem Advanced Materials and 99.999% purity CuI powders from Sigma-Aldrich were used as starting materials. A CsCu_2I_3 single crystal with a 7 mm diameter was grown by the vertical Bridgman method. These starting materials were weighted according to the stoichiometric ratio, and then mixed and loaded into a 7 mm diameter quartz ampoule in a glovebox with <0.1 ppm moisture and <0.1 ppm oxygen. Before loading raw materials, the quartz ampoule was cleaned with deionized water and acetone to remove impurities on the inner surface before loading raw materials. Then, the loaded ampoule was dried at 180°C for 16 hours under a vacuum degree of 10^{-6} torr to remove residual water and oxygen impurities. After drying treatment, the ampoule was sealed and placed into a Bridgman growth furnace. Prior to crystal growth, the CsCu_2I_3 compound was pre-synthesized at 630°C for 24 hours. The actual growth started at 383°C and used a temperature gradient of $20\text{--}30^\circ\text{C/cm}$ and a pulling rate of $0.5\text{--}1\text{ mm/h}$. The furnace temperature was then cooled with a rate of 10°C/h to room temperature by the end of crystal growth.

Single crystal X-ray diffraction measurement

To collect the single-crystal X-ray diffraction data, a single crystal of CsCu_2I_3 was mounted on a Bruker D8 VENTURE Diffractometer with $\text{Mo } K_\alpha$ radiation ($\lambda = 0.71073\text{ \AA}$) at room temperature. The data reduction and multiscan absorption correction were performed using the CrysAlis Pro v. 171.37.33

software. The structure was solved with the direct methods algorithm using the program ShelXS, and refined against F^2 using the program ShelXL.

Differential thermal analysis (DTA) measurement

The DTA measurement was performed on a Netzsch STA449F3 instrument. A CsCu_2I_3 single crystal sample about 50 mg was placed in a Al_2O_3 crucible. Then, the loaded crucible was heated and cooled with a speed of 5 K/min under the ultra-high purity Ar gas flow. A baseline was obtained by measuring an empty sample crucible pan under identical conditions.

Hygroscopicity measurements

Moisture sorption profiles of a cylindrical CsCu_2I_3 single crystal sample was measured by recording weight changes at 25°C for 4 hours under a relative humidity of 80%. A cylindrical NaI:Tl crystal sample with same surface area was also measured for comparison.

Optical and scintillation property measurements

Optical absorption spectrum was measured using a Shimadzu 3101PC spectrometer. Photoluminescence excitation (PLE) and emission (PL) contour mapping were measured with Horiba FluoroMax+ spectrofluorometer equipped with a Xe lamp and dual scanning monochromators. PL and PLE spectra, radioluminescence (RL) spectra and PL decays were acquired using a custom-made spectrofluorometer 5000M (Horiba Jobin Yvon), with a steady state laser-driven xenon lamp (PL and PLE spectra, Energetiq EQ-99X LDLS - Hamamatsu), X-ray tube with Mo anode (RL spectra, 40 kV, 15 mA, Seifert

GmbH), and nanosecond pulsed nanoLED light sources (PL decay curves, Horiba) as the excitation sources. X-ray induced afterglow profile was measured with the custom-made spectrofluorometer 5000M and a X-ray excitation source described above.

The absolute light yield and energy resolution was measured by pulse height spectra using the set-up consisting of a Hamamatsu R2059 PMT with preamplifier, measuring electronics using Ortec 672 Spectroscopy Amplifier with a MCA and personal computer control. A shaping time of 10 μ s was used to provide light integration.

RESULTS AND DISCUSSION

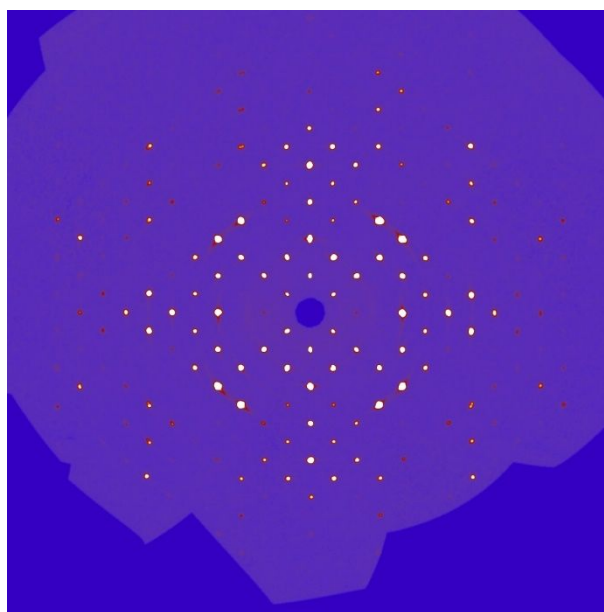


Figure S1. *hk0* precession pattern of CsCu₂I₃.

Table S1. Selected crystallographic data and structure refinement for CsCu₂I₃.

Formula	CsCu ₂ I ₃
Fw (g mol ⁻¹)	640.69
<i>T</i> (K)	293(2)
Space group	<i>Cmcm</i> (No. 63)
<i>a</i> (Å)	10.5583(7)
<i>b</i> (Å)	13.1912(9)
<i>c</i> (Å)	6.1032(4)
<i>Z</i>	4
<i>D</i> _{calc} (mg m ⁻³)	5.006
μ (Mo Ka) (mm ⁻¹)	20.013
<i>F</i> (000)	1088
θ range for data collection (°)	2.471-26.334
No. of reflections (all)	507
No. of reflections (obs)	445
No. of parameters	20
<i>R</i> _{obs} , <i>wR</i> _{obs}	0.0255, 0.0592
<i>R</i> _{all} , <i>wR</i> _{all}	0.0302, 0.0614
Goodness of fit	1.142
Max. / Min. residual electrostatic potential (e Å ⁻³)	1.146, -1.395

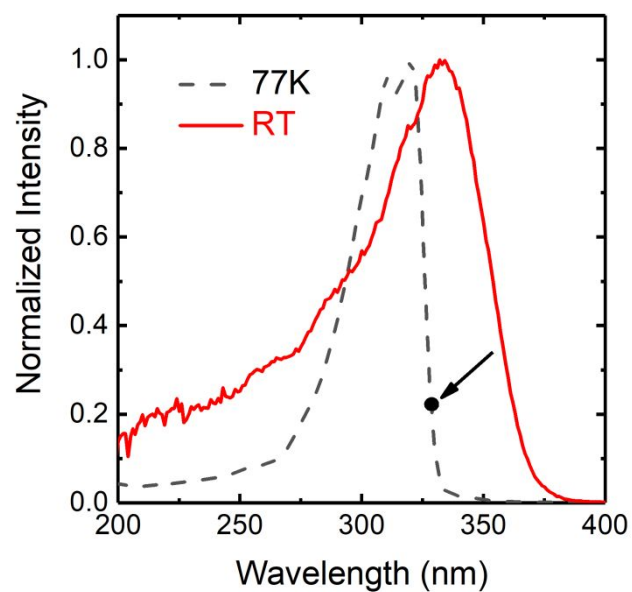


Figure S2. The photoluminescence excitation spectra of CsCu₂I₃ measured at 77 and 300 K monitoring emission wavelength of 560 nm.

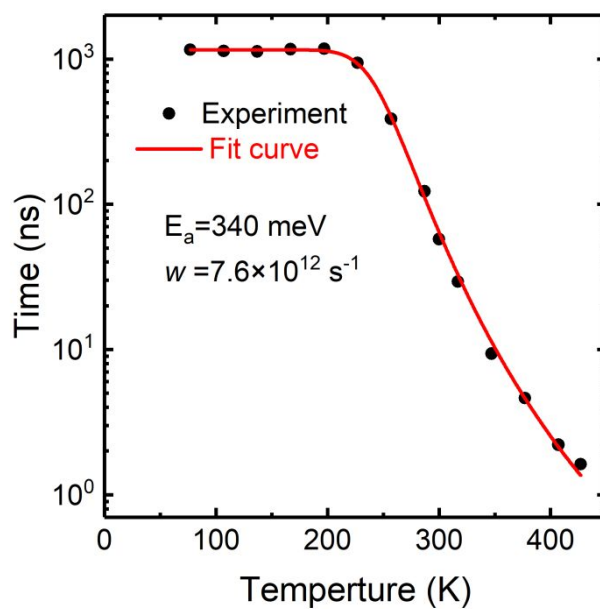


Figure S3. The PL decays as a functional of temperature from 77 to 447 K. The fitting results of activation energy and frequency factor are shown in inset.