

Support Information

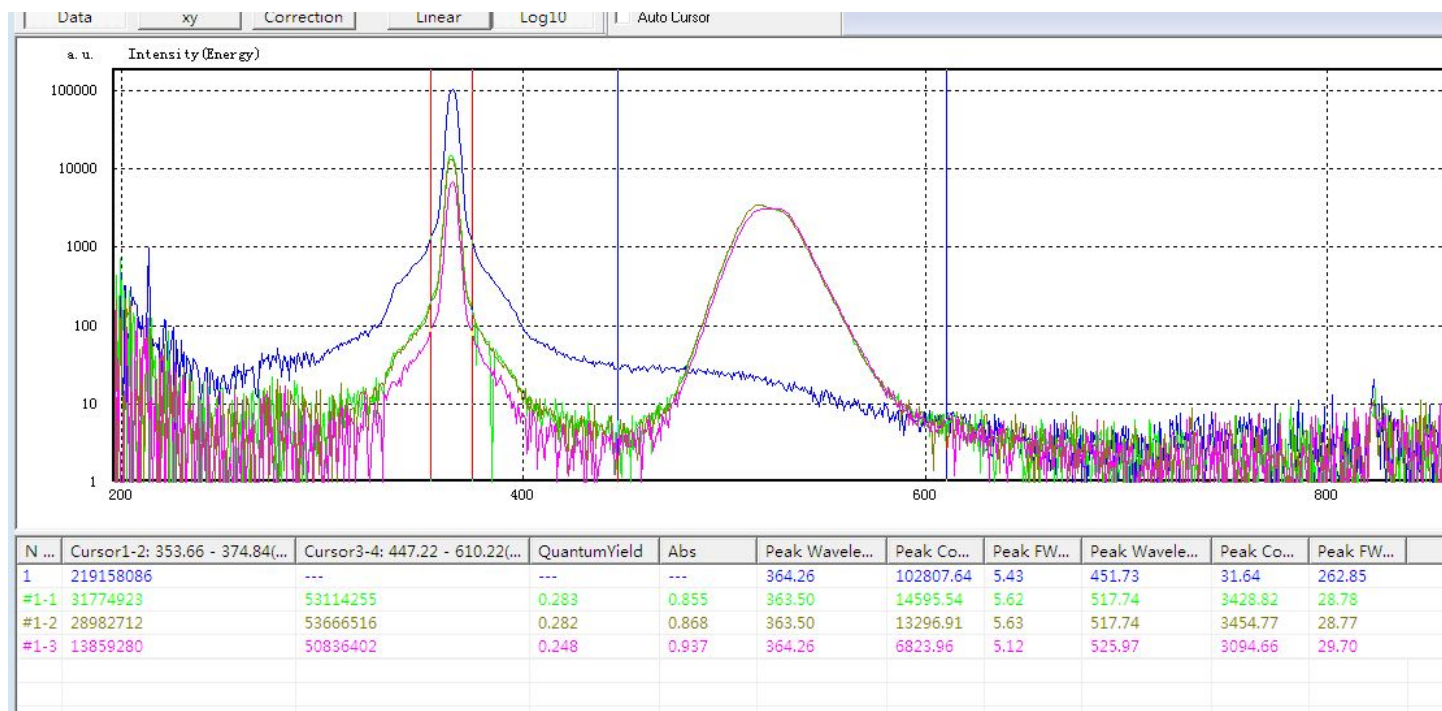
Influence of Lewis Basicity on the S²⁻ Induced Synthesis of 0D Cs₄PbBr₆ Hexagonal Nanocrystals and Its Implications for Optoelectronics

Yukun Liu, Yangai Liu,* Chenguang Yang, Lefu Mei, Hao Ding, Ruiyu Mi, and Yuanyuan Zhang*

^aBeijing Key Laboratory of Material Utilization of Nonmetallic Minerals and Solid Wastes, National Laboratory of Mineral Materials, School of Materials Sciences and Technology, China University of Geosciences, Beijing 100083, China.

^bSchool of Materials Sciences and Technology, Dongguan University of Technology, Dongguan 523808, China.

Quantaaurus-QY Plus C13534-12 and Hamamatsu Photonics were used to measure the quantum yield of the sample. LED test instrument: Hangzhou Hopoo Light&Color Technology Co.,Ltd.OHSP-350M LED Fast-Scan Spectrophotometer (350-1050nm).



These are Cs₄PbBr₆ HNCs package LED OHSP test report:

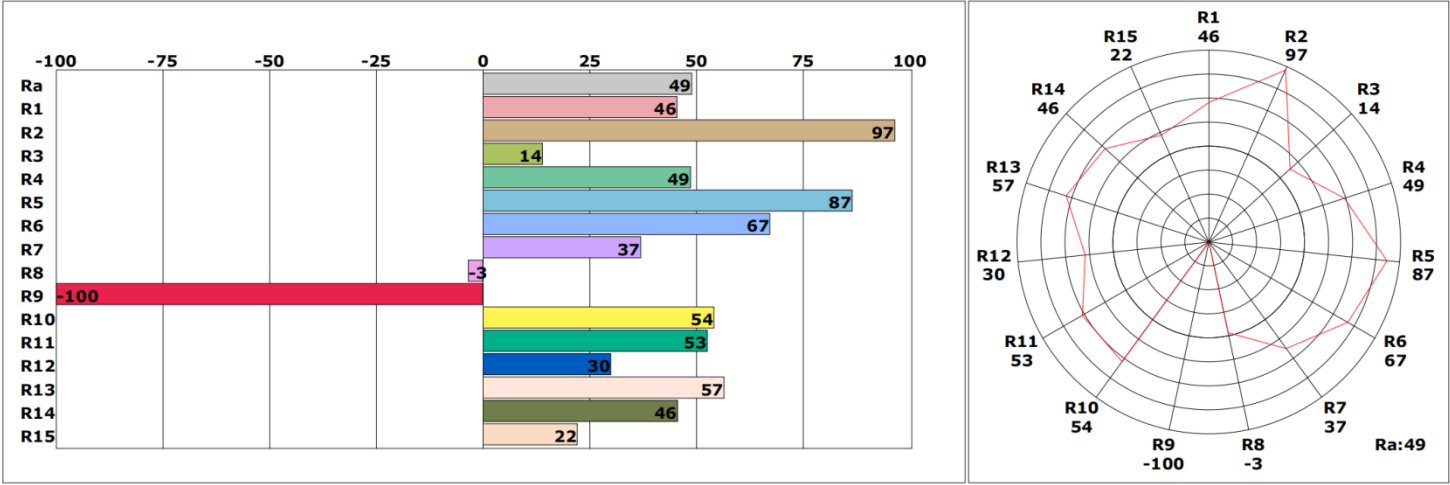
OHSP Test Report

Parameter Name	Parameter Value	Parameter Name	Parameter Value	Parameter Name	Parameter Value	Parameter Name	Parameter Value
Luminous Flux (lm)	0.23	Color Purity (%)	6.9	Φ _{er} (mW)	0.266	K _{ppfv} (μmol/s/klm)	14.826
Luminous Efficacy (lm/W)	4.47	FWHM (nm)	9.2	Φ _{eu} v(mW)	0.000	Y _{PF} (μmol/s)	0.003
Correlated Color Temperature (K)	6410	Peak Wavelength (nm)	630.1	Φ _{efr} (mW)	0.000	Φ _{ep} (mW)	0.646
Blackbody Deviation Duv	-0.00053	Center Wavelength (nm)	630.9	Φ _{eir} (mW)	0.000	Integration Time (ms)	320
Chromaticity Coordinates (x, y)	0.3151,0.3242	Centroid Wavelength (nm)	543.7	Φ _{ec} (mW)	0.000	Peak Signal	51492
Chromaticity Coordinates (u, v)	0.2013,0.3107	Luminous Flux Ratio (RGB)	24.3,72.8,2.9	Φ _{erb} Ratio	1.183	Dark Signal	3238
Chromaticity Coordinates (u', v')	0.2013,0.4661	CIE1931 X	0.331	P _{AR} (mW)	0.759	Compensation Level	2824
Color Difference	9.96	CIE1931 Y	0.341	E _{chA} (mW)	0.000	Voltage (V)	2.624
Color Rendering Index (Ra)	49.0	CIE1931 Z	0.379	E _{chB} (mW)	0.000	Current (A)	0.020
Radiant Flux (mW)	0.757	TLCI-2012	8	P _{PF} (umol/s)	0.003	Power (W)	0.052
Blue Light Hazard Irradiance (mW)	0.00	Flicker Frequency (Hz)	0.00	P _{PF_UV} (umol/s)	0.000	Power Factor	0.000
B _{ck} (μW/lm)	0.88	Modulation Depth (%)	0.0	P _{PF_B} (umol/s)	0.001		
Scotopic/Photopic Ratio (S/P)	2.084	Flicker Percentage (%)	0.0	P _{PF_G} (umol/s)	0.001		
Fidelity Index (R _f)	56.97	Flicker Index	0.00	P _{PF_R} (umol/s)	0.001		
Gamut Index (R _g)	124.51	Φ _{eb} (mW)	0.225	P _{PF_FR} (umol/s)	0.000		
Dominant Wavelength (nm)	485.00	Φ _{ey} (mW)	0.268	P _{PF_IR} (umol/s)	0.000		

Spectrogram

CIE1931

Color rendering index



Instrument Status

Instrument Model: OHSP-350M

Peak Signal: 51492

Integration Time: 320.000 ms

Wavelength Range: 350-800 nm

Instrument Serial Number: 352107863

Dark Voltage: 3238

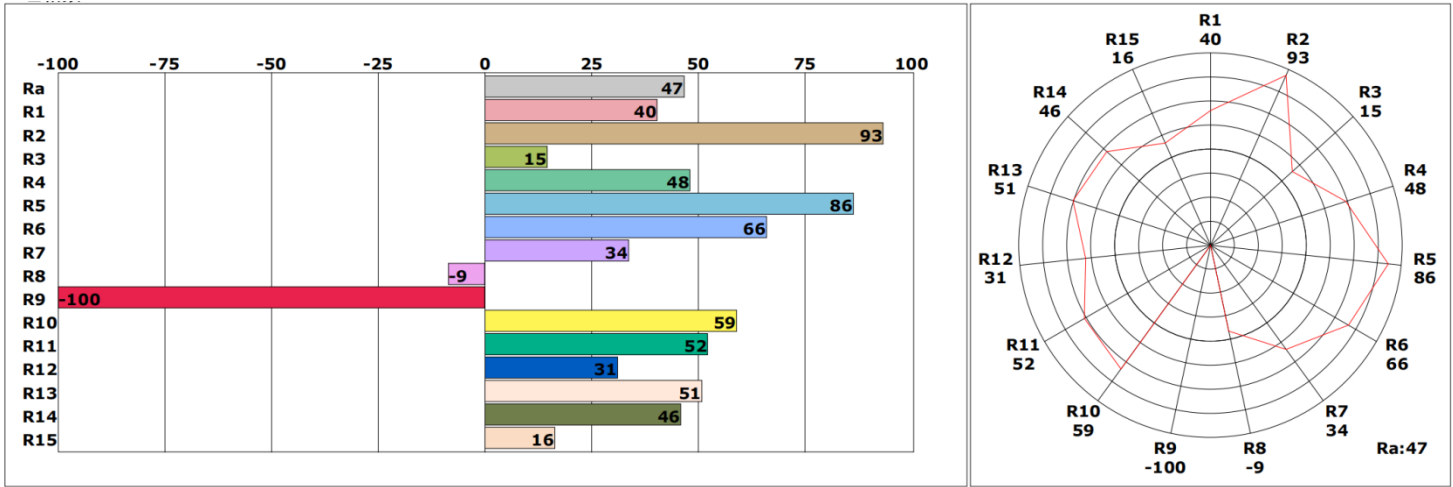
OHSP Test Report

Parameter Name	Parameter Value	Parameter Name	Parameter Value	Parameter Name	Parameter Value	Parameter Name	Parameter Value
Luminous Flux (lm)	0.46	Color Purity (%)	7.0	$\Phi_{er}(mW)$	0.528	$K_{ppfv}(\mu mol/s/klm)$	14.831
Luminous Efficacy (lm/W)	4.32	FWHM (nm)	8.9	$\Phi_{euv}(mW)$	0.000	YPF ($\mu mol/s$)	0.006
Correlated Color Temperature (K)	6382	Peak Wavelength (nm)	630.1	$\Phi_{efr}(mW)$	0.000	$\Phi_{ep}(mW)$	1.274
Blackbody Deviation Duv	-0.00317	Center Wavelength (nm)	631.0	$\Phi_{eir}(mW)$	0.000	Integration Time (ms)	160
Chromaticity Coordinates (x, y)	0.3161,0.3201	Centroid Wavelength (nm)	543.6	$\Phi_{ec}(mW)$	0.000	Peak Signal	50691
Chromaticity Coordinates (u, v)	0.2036,0.3093	Luminous Flux Ratio (RGB)	24.9,72.2,2.9	$\Phi_{erb}Ratio$	1.180	Dark Signal	2491
Chromaticity Coordinates (u', v')	0.2036,0.4640	CIE1931 X	0.662	PAR(mW)	1.494	Compensation Level	2824
Color Difference	13.32	CIE1931 Y	0.670	EchA(mW)	0.000	Voltage (V)	2.670
Color Rendering Index (Ra)	46.8	CIE1931 Z	0.761	EchB(mW)	0.000	Current (A)	0.040
Radiant Flux (mW)	1.503	TLCI-2012	10	PPF(umol/s)	0.007	Power (W)	0.106
Blue Light Hazard Irradiance (mW)	0.00	Flicker Frequency (Hz)	0.00	PPF_UV(umol/s)	0.000	Power Factor	0.000
Bek ($\mu W/lm$)	0.89	Modulation Depth (%)	59.9	PPF_B(umol/s)	0.002		
Scotopic/Photopic Ratio (S/P)	2.079	Flicker Percentage (%)	42.8	PPF_G(umol/s)	0.002		
Fidelity Index (Rf)	55.94	Flicker Index	0.21	PPF_R(umol/s)	0.003		
Gamut Index (Rg)	126.01	$\Phi_{eb}(mW)$	0.448	PPF_FR(umol/s)	0.000		
Dominant Wavelength (nm)	481.10	$\Phi_{ey}(mW)$	0.517	PPF_IR(umol/s)	0.000		

Spectrogram

CIE1931

Color rendering index



Instrument Status

Instrument Model: OHSP-350M

Peak Signal: 50691

Integration Time: 160.000 ms

Wavelength Range: 350-800 nm

Instrument Serial Number: 352107863

Dark Voltage: 2491

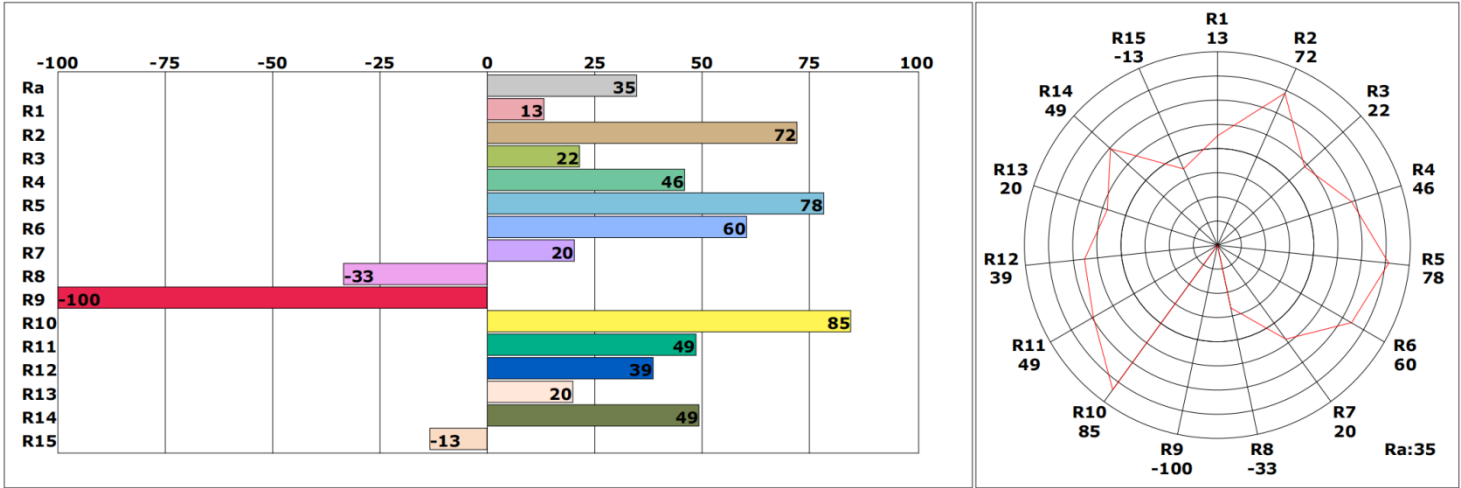
OHSP Test Report

Parameter Name	Parameter Value	Parameter Name	Parameter Value	Parameter Name	Parameter Value	Parameter Name	Parameter Value
Luminous Flux (lm)	0.63	Color Purity (%)	11.1	$\Phi_{er}(mW)$	0.806	Kppfv ($\mu mol/s/klm$)	15.925
Luminous Efficacy (lm/W)	3.92	FWHM (nm)	9.2	$\Phi_{euv}(mW)$	0.000	YPF ($\mu mol/s$)	0.009
Correlated Color Temperature (K)	6505	Peak Wavelength (nm)	630.1	$\Phi_{efr}(mW)$	0.000	$\Phi_{ep}(mW)$	1.880
Blackbody Deviation Duv	-0.01726	Center Wavelength (nm)	631.1	$\Phi_{eir}(mW)$	0.000	Integration Time (ms)	110
Chromaticity Coordinates (x, y)	0.3173,0.2963	Centroid Wavelength (nm)	541.8	$\Phi_{ec}(mW)$	0.000	Peak Signal	51674
Chromaticity Coordinates (u, v)	0.2144,0.3002	Luminous Flux Ratio (RGB)	28.1,68.5,3.4	Φ_{erb} Ratio	1.103	Dark Signal	2223
Chromaticity Coordinates (u', v')	0.2144,0.4504	CIE1931 X	0.983	PAR(mW)	2.204	Compensation Level	2824
Color Difference	21.60	CIE1931 Y	0.918	EchA(mW)	0.000	Voltage (V)	2.705
Color Rendering Index (Ra)	34.9	CIE1931 Z	1.197	EchB(mW)	0.000	Current (A)	0.059
Radiant Flux (mW)	2.199	TLCI-2012	1	PPF($\mu mol/s$)	0.010	Power (W)	0.160
Blue Light Hazard Irradiance (mW)	0.00	Flicker Frequency (Hz)	0.00	PPF_UV($\mu mol/s$)	0.000	Power Factor	0.000
Bck ($\mu W/lm$)	1.06	Modulation Depth (%)	59.9	PPF_B($\mu mol/s$)	0.003		
Scotopic/Photopic Ratio (S/P)	2.157	Flicker Percentage (%)	42.8	PPF_G($\mu mol/s$)	0.003		
Fidelity Index (Rf)	51.75	Flicker Index	0.00	PPF_R($\mu mol/s$)	0.004		
Gamut Index (Rg)	132.50	$\Phi_{eb}(mW)$	0.731	PPF_FR($\mu mol/s$)	0.000		
Dominant Wavelength (nm)	380.00	$\Phi_{ey}(mW)$	0.667	PPF_IR($\mu mol/s$)	0.000		

Spectrogram

CIE1931

Color rendering index



Instrument Status

Instrument Model: OHSP-350M

Integration Time: 110.000 ms

Instrument Serial Number: 352107863

Peak Signal: 51674

Wavelength Range: 350-800 nm

Dark Voltage: 2223

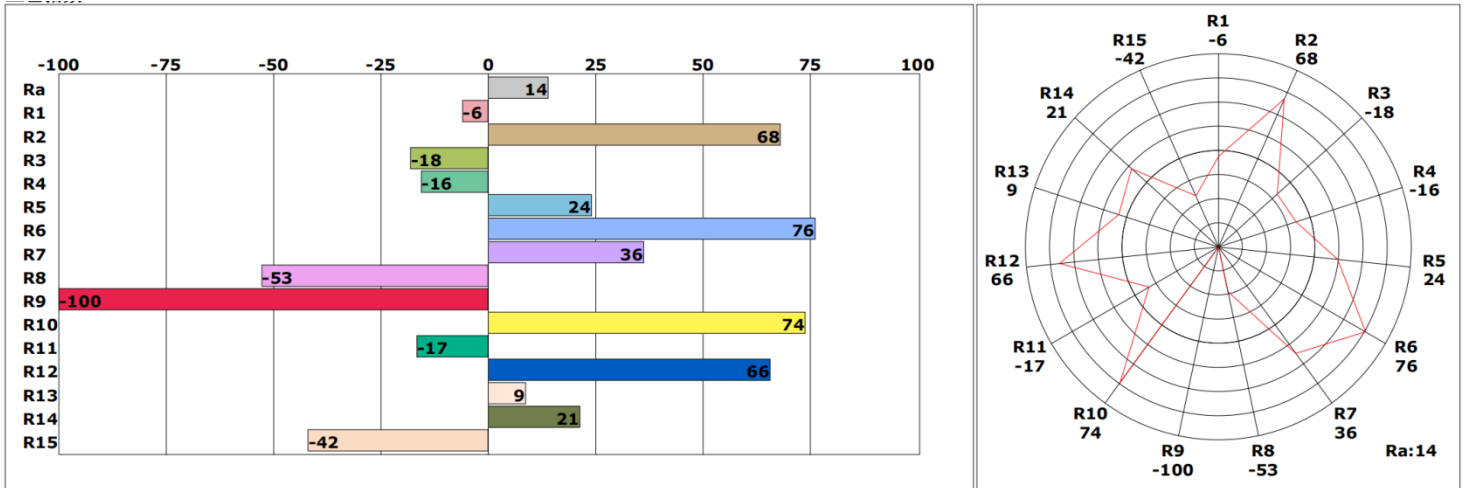
OHSP Test Report

Parameter Name	Parameter Value	Parameter Name	Parameter Value	Parameter Name	Parameter Value	Parameter Name	Parameter Value
Luminous Flux (lm)	0.69	Color Purity (%)	34.5	$\Phi_{er}(mW)$	1.083	Kppfv (μmol/s/klm)	18.824
Luminous Efficacy (lm/W)	3.19	FWHM (nm)	9.5	$\Phi_{euv}(mW)$	0.000	YPF (μmol/s)	0.011
Correlated Color Temperature (K)	8712	Peak Wavelength (nm)	630.1	$\Phi_{efr}(mW)$	0.000	$\Phi_{ep}(mW)$	2.464
Blackbody Deviation Duv	-0.05070	Center Wavelength (nm)	631.0	$\Phi_{eir}(mW)$	0.000	Integration Time (ms)	85
Chromaticity Coordinates (x, y)	0.3121,0.2402	Centroid Wavelength (nm)	537.5	$\Phi_{ec}(mW)$	0.000	Peak Signal	52932
Chromaticity Coordinates (u, v)	0.2374,0.2741	Luminous Flux Ratio (RGB)	33.2,62.3,4.5	Φ_{erb} Ratio	0.966	Dark Signal	2469
Chromaticity Coordinates (u', v')	0.2374,0.4111	CIE1931 X	1.316	PAR(mW)	2.897	Compensation Level	2830
Color Difference	43.31	CIE1931 Y	1.013	EchA(mW)	0.000	Voltage (V)	2.736
Color Rendering Index (Ra)	14.0	CIE1931 Z	1.887	EchB(mW)	0.000	Current (A)	0.079
Radiant Flux (mW)	2.897	TLCI-2012	27	PPF(umol/s)	0.013	Power (W)	0.217
Blue Light Hazard Irradiance (mW)	0.00	Flicker Frequency (Hz)	0.00	PPF_UV(umol/s)	0.000	Power Factor	0.000
Bek (μW/lm)	1.47	Modulation Depth (%)	0.0	PPF_B(umol/s)	0.004		
Scotopic/Photopic Ratio (S/P)	2.355	Flicker Percentage (%)	0.0	PPF_G(umol/s)	0.003		
Fidelity Index (Rf)	40.23	Flicker Index	0.00	PPF_R(umol/s)	0.006		
Gamut Index (Rg)	141.05	$\Phi_{eb}(mW)$	1.121	PPF_FR(umol/s)	0.000		
Dominant Wavelength (nm)	563.00	$\Phi_{ey}(mW)$	0.694	PPF_IR(umol/s)	0.000		

Spectrogram

CIE1931

Color rendering index



Instrument Status

Instrument Model: OHSP-350M

Integration Time: 85.000 ms

Instrument Serial Number: 352107863

Peak Signal: 52932

Wavelength Range: 350-800 nm

Dark Voltage: 2469

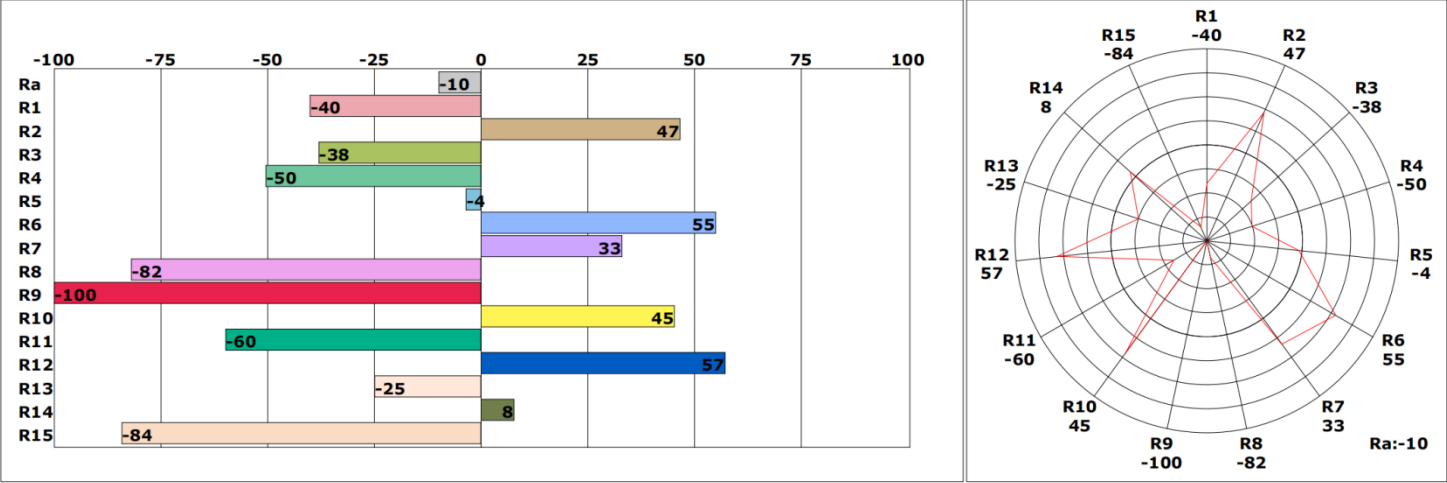
OHSP Test Report

Parameter Name	Parameter Value	Parameter Name	Parameter Value	Parameter Name	Parameter Value	Parameter Name	Parameter Value
Luminous Flux (lm)	0.75	Color Purity (%)	47.2	$\Phi_{er}(mW)$	1.367	Kppfv ($\mu mol/s/klm$)	21.481
Luminous Efficacy (lm/W)	2.74	FWHM (nm)	9.2	$\Phi_{euv}(mW)$	0.000	YPF ($\mu mol/s$)	0.014
Correlated Color Temperature (K)	23450	Peak Wavelength (nm)	630.1	$\Phi_{efr}(mW)$	0.000	$\Phi_{ep}(mW)$	3.075
Blackbody Deviation Duv	-0.07402	Center Wavelength (nm)	631.1	$\Phi_{eir}(mW)$	0.000	Integration Time (ms)	67
Chromaticity Coordinates (x, y)	0.3065,0.2036	Centroid Wavelength (nm)	533.2	$\Phi_{ec}(mW)$	0.000	Peak Signal	52431
Chromaticity Coordinates (u, v)	0.2538,0.2529	Luminous Flux Ratio (RGB)	38.5,55.6,5.8	Φ_{erb} Ratio	0.864	Dark Signal	2393
Chromaticity Coordinates (u', v')	0.2538,0.3794	CIE1931 X	1.659	PAR(mW)	3.627	Compensation Level	2830
Color Difference	57.95	CIE1931 Y	1.102	EchA(mW)	0.000	Voltage (V)	2.765
Color Rendering Index (Ra)	-9.9	CIE1931 Z	2.651	EchB(mW)	0.000	Current (A)	0.100
Radiant Flux (mW)	3.627	TLCI-2012	28	PPF($\mu mol/s$)	0.016	Power (W)	0.275
Blue Light Hazard Irradiance (mW)	0.00	Flicker Frequency (Hz)	0.00	PPF_UV($\mu mol/s$)	0.000	Power Factor	0.000
Bek ($\mu W/lm$)	1.90	Modulation Depth (%)	0.0	PPF_B($\mu mol/s$)	0.006		
Scotopic/Photopic Ratio (S/P)	2.586	Flicker Percentage (%)	0.0	PPF_G($\mu mol/s$)	0.003		
Fidelity Index (Rf)	25.18	Flicker Index	0.00	PPF_R($\mu mol/s$)	0.007		
Gamut Index (Rg)	149.29	$\Phi_{eb}(mW)$	1.582	PPF_FR($\mu mol/s$)	0.000		
Dominant Wavelength (nm)	562.40	$\Phi_{ey}(mW)$	0.678	PPF_IR($\mu mol/s$)	0.000		

Spectrogram

CIE1931

Color rendering index



Instrument Status

Instrument Model: OHSP-350M

Peak Signal: 52431

Integration Time: 67.000 ms

Wavelength Range: 350-800 nm

Instrument Serial Number: 352107863

Dark Voltage: 2393

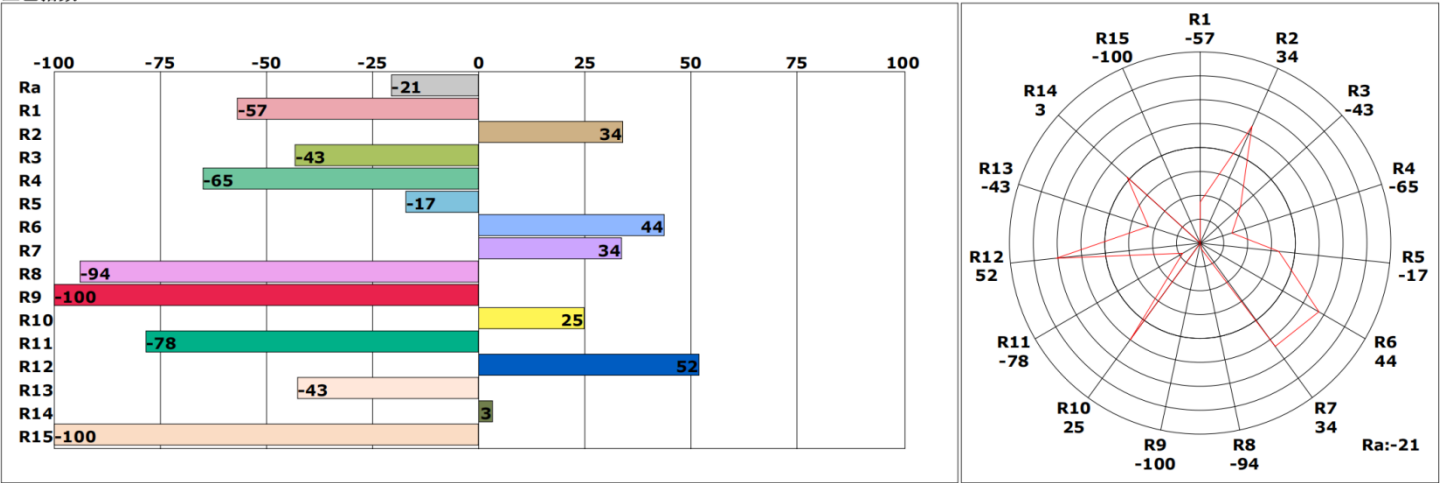
OHSP Test Report

Parameter Name	Parameter Value	Parameter Name	Parameter Value	Parameter Name	Parameter Value	Parameter Name	Parameter Value
Luminous Flux (lm)	0.83	Color Purity (%)	52.1	$\Phi_{er}(mW)$	1.643	Kppfv ($\mu mol/s/klm$)	22.881
Luminous Efficacy (lm/W)	2.49	FWHM (nm)	9.2	$\Phi_{euv}(mW)$	0.000	YPF ($\mu mol/s$)	0.017
Correlated Color Temperature (K)	100000	Peak Wavelength (nm)	630.1	$\Phi_{efr}(mW)$	0.000	$\Phi_{ep}(mW)$	3.642
Blackbody Deviation Duv	-0.08532	Center Wavelength (nm)	631.1	$\Phi_{eir}(mW)$	0.000	Integration Time (ms)	56
Chromaticity Coordinates (x, y)	0.3057,0.1885	Centroid Wavelength (nm)	531.9	$\Phi_{ec}(mW)$	0.000	Peak Signal	52566
Chromaticity Coordinates (u, v)	0.2629,0.2432	Luminous Flux Ratio (RGB)	41.9,51.6,6.4	$\Phi_{erb}Ratio$	0.841	Dark Signal	2324
Chromaticity Coordinates (u', v')	0.2629,0.3648	CIE1931 X	1.982	PAR(mW)	4.296	Compensation Level	2830
Color Difference	64.47	CIE1931 Y	1.222	EchA(mW)	0.000	Voltage (V)	2.794
Color Rendering Index (Ra)	-20.5	CIE1931 Z	3.279	EchB(mW)	0.000	Current (A)	0.120
Radiant Flux (mW)	4.296	TLCI-2012	28	PPF($\mu mol/s$)	0.019	Power (W)	0.335
Blue Light Hazard Irradiance (mW)	0.00	Flicker Frequency (Hz)	0.00	PPF_UV($\mu mol/s$)	0.000	Power Factor	0.000
Bek ($\mu W/lm$)	2.12	Modulation Depth (%)	0.0	PPF_B($\mu mol/s$)	0.007		
Scotopic/Photopic Ratio (S/P)	2.682	Flicker Percentage (%)	0.0	PPF_G($\mu mol/s$)	0.003		
Fidelity Index (Rf)	17.00	Flicker Index	0.00	PPF_R($\mu mol/s$)	0.009		
Gamut Index (Rg)	154.00	$\Phi_{eb}(mW)$	1.954	PPF_FR($\mu mol/s$)	0.000		
Dominant Wavelength (nm)	561.90	$\Phi_{ey}(mW)$	0.698	PPF_IR($\mu mol/s$)	0.000		

Spectrogram

CIE1931

Color rendering index



Instrument Status

Instrument Model: OHSP-350M

Peak Signal: 52566

Integration Time: 56.000 ms

Wavelength Range: 350-800 nm

Instrument Serial Number: 352107863

Dark Voltage: 2324

To determine the content of elements Cs, Pb, Br, and S in the prepared Cs₄PbBr₆ samples, we supplemented our analysis with ICP-MS testing. The table below presents the test data, including the concentrations of elements measured multiple times. The average elemental content of the samples was calculated, and the consistency of the data was evaluated.

The test results indicate a low S content, which aligns with our expectations. This is because only 0.07 mol% of PbS was introduced during the synthesis process, and a certain amount was removed during centrifugation and purification. In contrast, the contents of Cs, Pb, and Br were relatively high, generally consistent with the stoichiometric ratio of Cs₄PbBr₆, though some discrepancies were observed. To identify the source of these discrepancies, we carefully reviewed the literature. Some studies have specifically investigated the use of ICP techniques for detecting halide perovskite quantum dots. They found that inductively coupled plasma (ICP), combined with conventional optical emission spectroscopy (OES) or mass spectrometry (MS) used for analyzing traditional metal chalcogenide nanocrystals (NCs), provides limited information for MHNCs. This is because significant errors can occur when detecting halides and organic ions. Consequently, the application of this technique is generally limited to measuring the doping levels of metal cations in NC systems, particularly when the dopant concentration is below 0.1%. Other techniques capable of detecting both cations and halide anions are therefore often preferred.

Table 1 ICP-MS test data of Cs₄PbBr₆

Sample Number	Sample Volume V(mL)	Final Volume V ₀ (mL)	Tested Element	Element Concentration in Testing Solution C ₀ (μg/L)	Dilution Factor f	Element Concentration in Digest Solution C ₁ (μg/L)	Element Content in Sample C _s (μg/L)
1	0.5	25	Pd	27.128	100	2712.758	135637.900
				28.067		2806.697	140334.850
				27.116		2711.580	135579.000
1	0.5	25	Cs	89.197	100	8919.686	445984.300
				91.075		9107.510	455375.500
				89.662		8966.175	448308.750
1	0.5	25	Br	163.291	200	32658.274	1632913.700
				165.714		33142.728	1657136.400

				169.173		33834.670	1691733.500
Sample Number	Sample Volume V(mL)	Final Volume V ₀ (mL)	Tested Element	Element Concentration in Testing Solution C ₀ (μg/L)	Dilution Factor f	Element Concentration in Digest Solution C _i (μg/L)	Element Content in Sample C _s (μg/L)
1	0.5	25	S	0.143	1	0.143	7.146
				0.157		0.157	7.834
				0.135		0.135	6.766
Instrument parameters	Pump Rate: 20r/min Nebulizer Flow: 1.00L/min Auxiliary Gas: 1.00L/min Sample Flush Time: 40s RF Power: 1550w						