Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Polarization-Sensitive Photodetection in A Two-Dimensional Interlayer-Multiple-Cation Hybrid Perovskite Bulk Single Crystal

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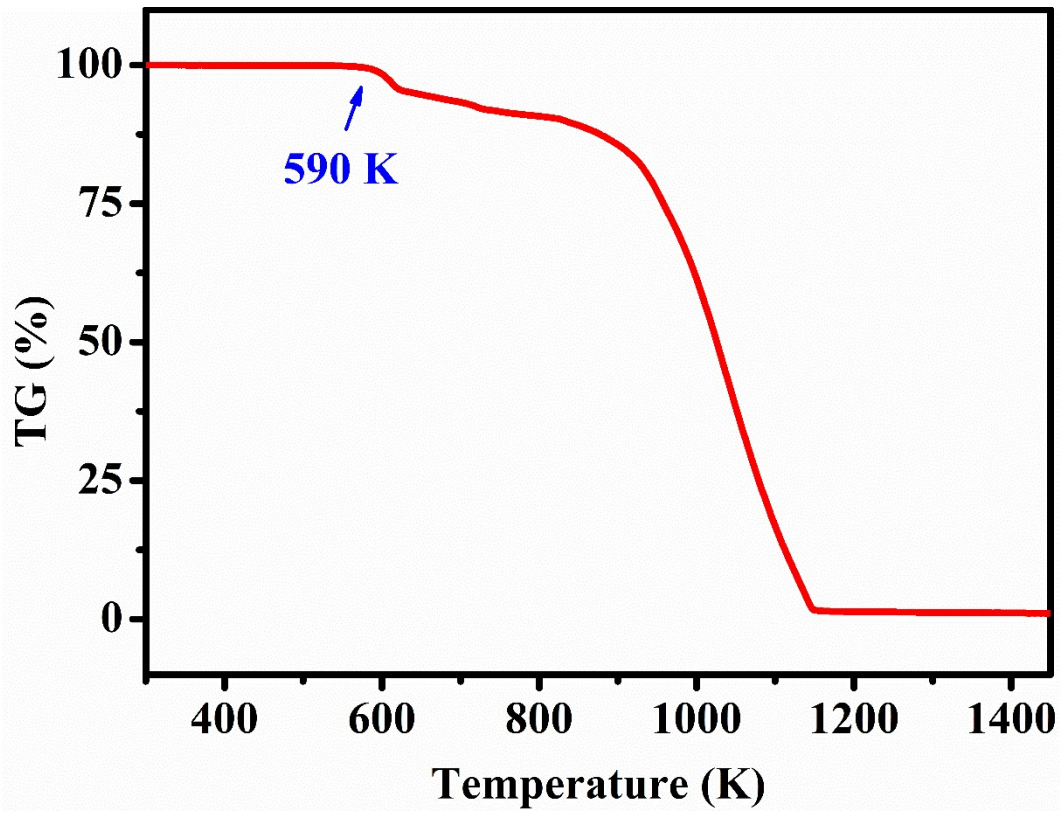

Figure S1. Thermogravimetric analysis of synthesized $Cs_2[C(NH_2)_3]Pb_2Br_7$

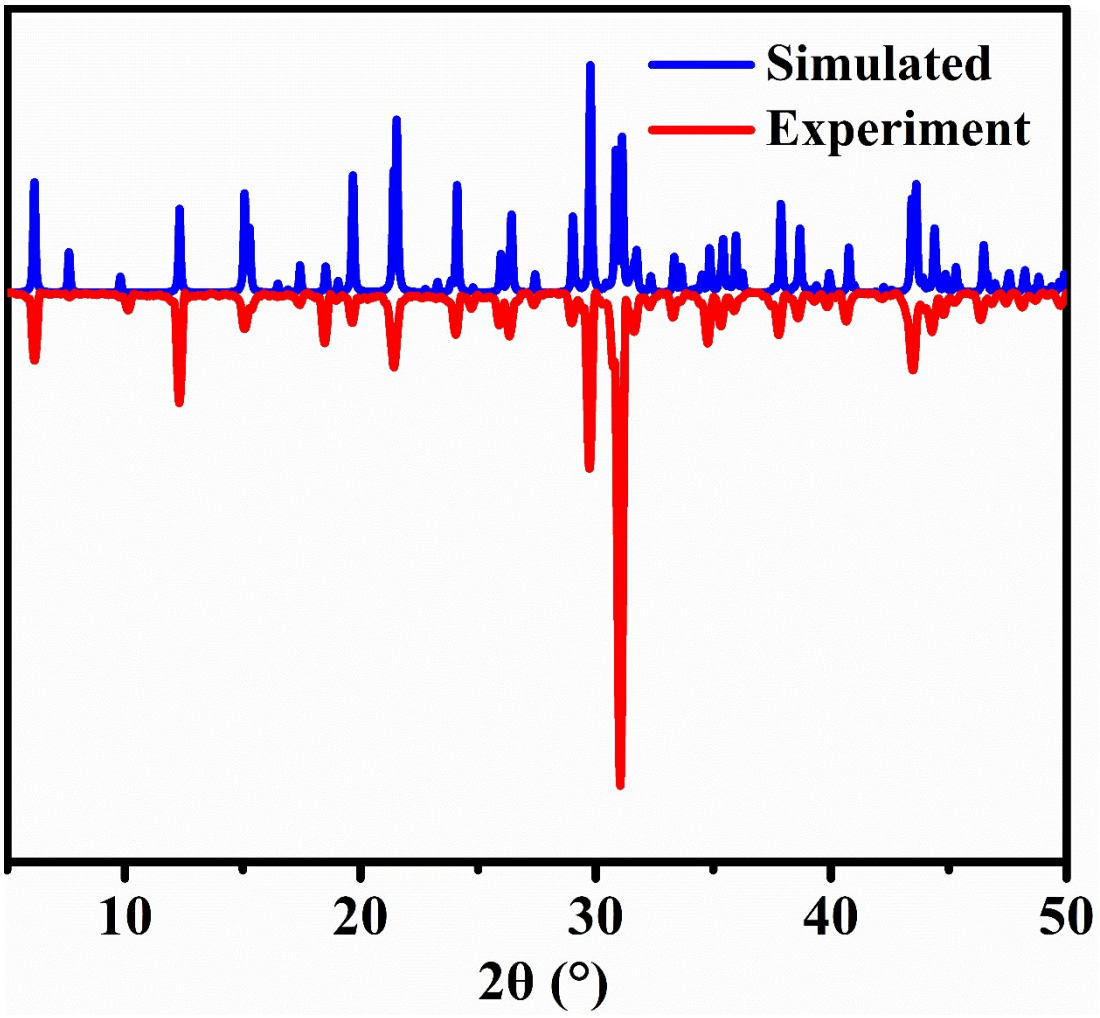

Figure S2. The simulated and experimental PXRD patterns of $Cs_2[C(NH_2)_3]Pb_2Br_7$

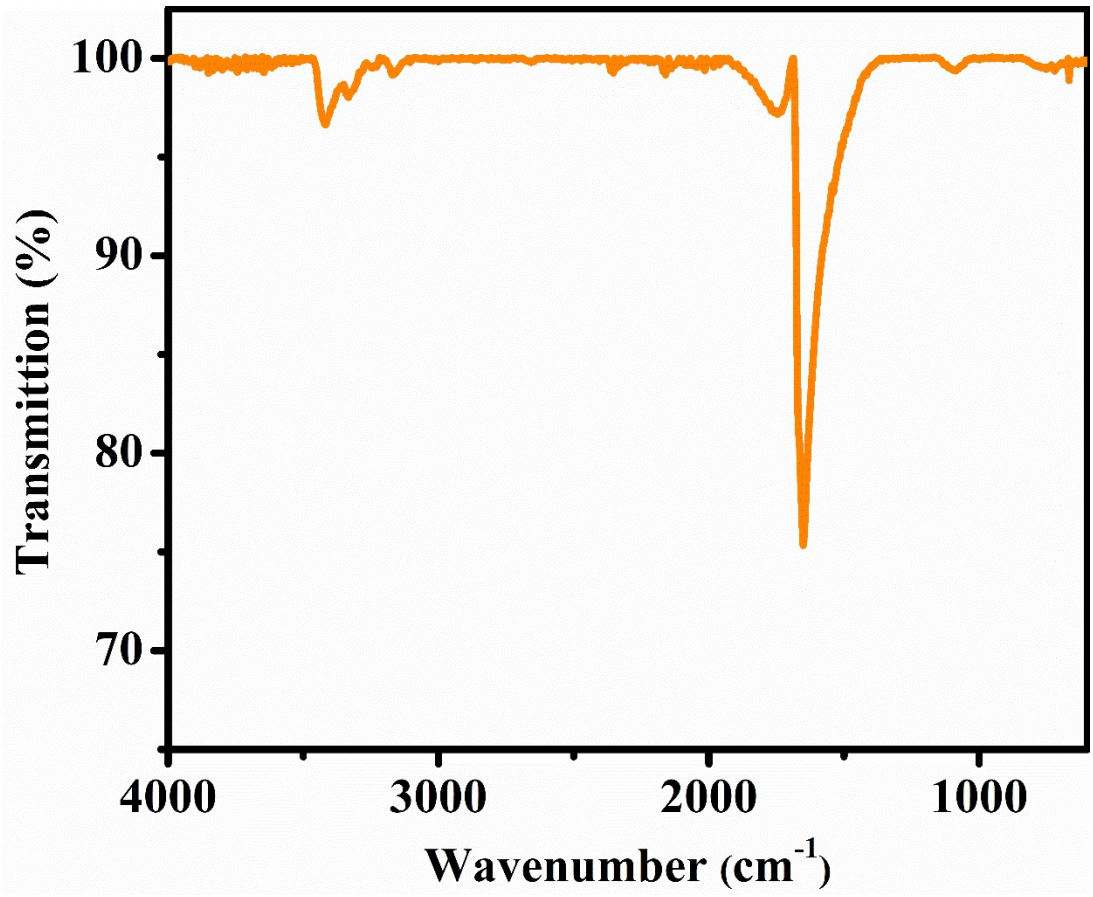

Figure S3. The IR spectrum of $Cs_2[C(NH_2)_3]Pb_2Br_7$

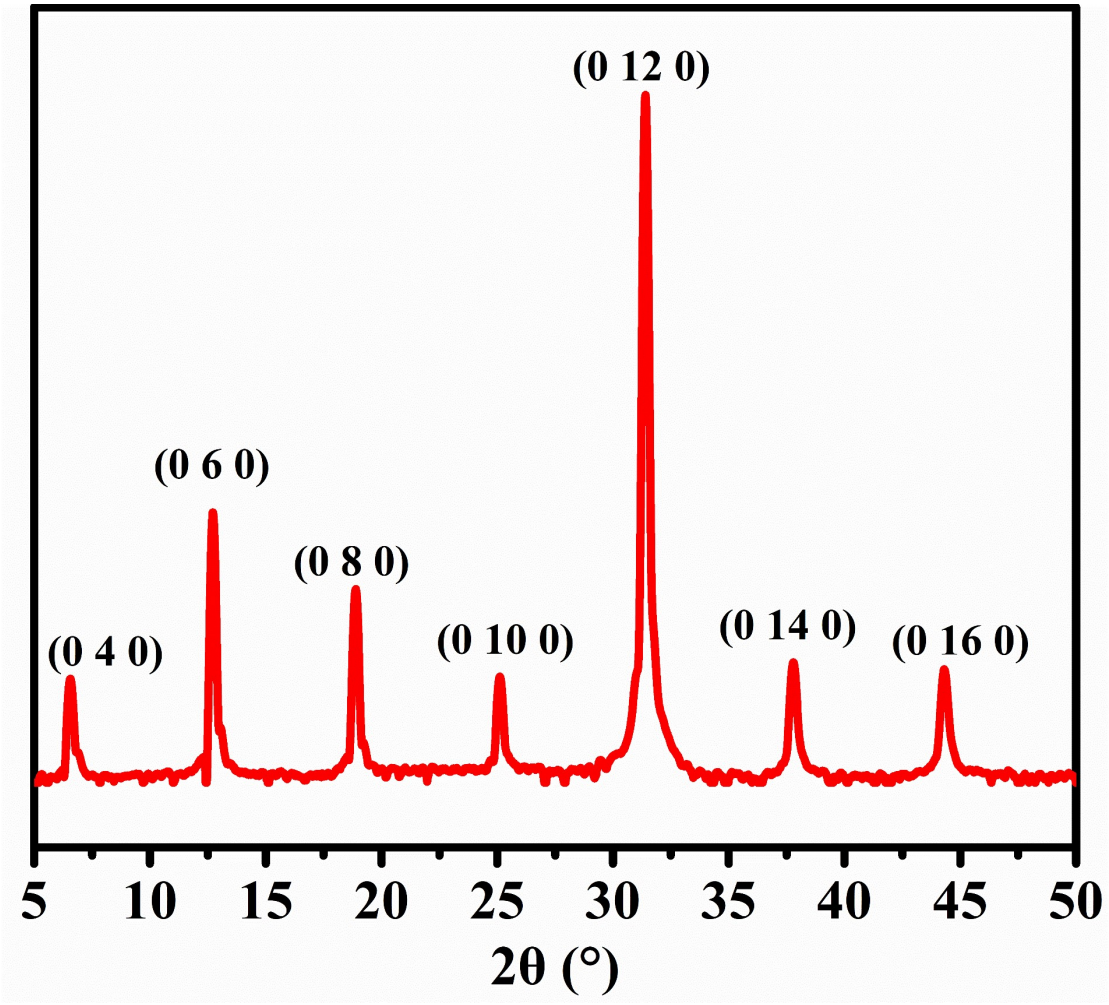

Figure S4. The PXRD patterns of single crystal $Cs_2[C(NH_2)_3]Pb_2Br_7$

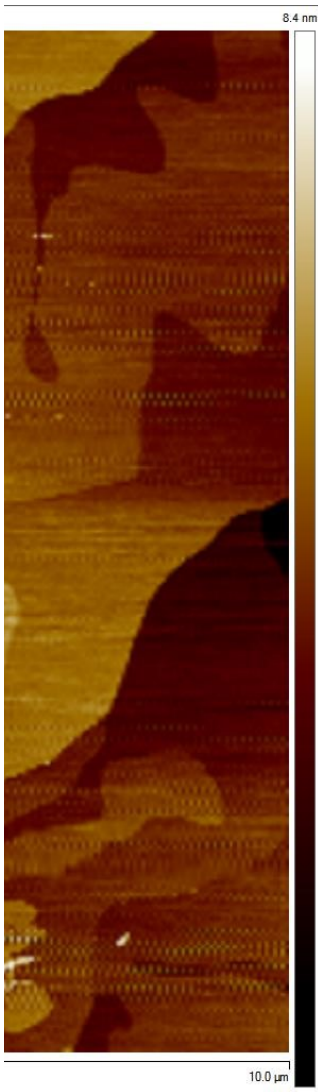

Figure S5. Atom force microscope test of single crystal $Cs_2[C(NH_2)_3]Pb_2Br_7$

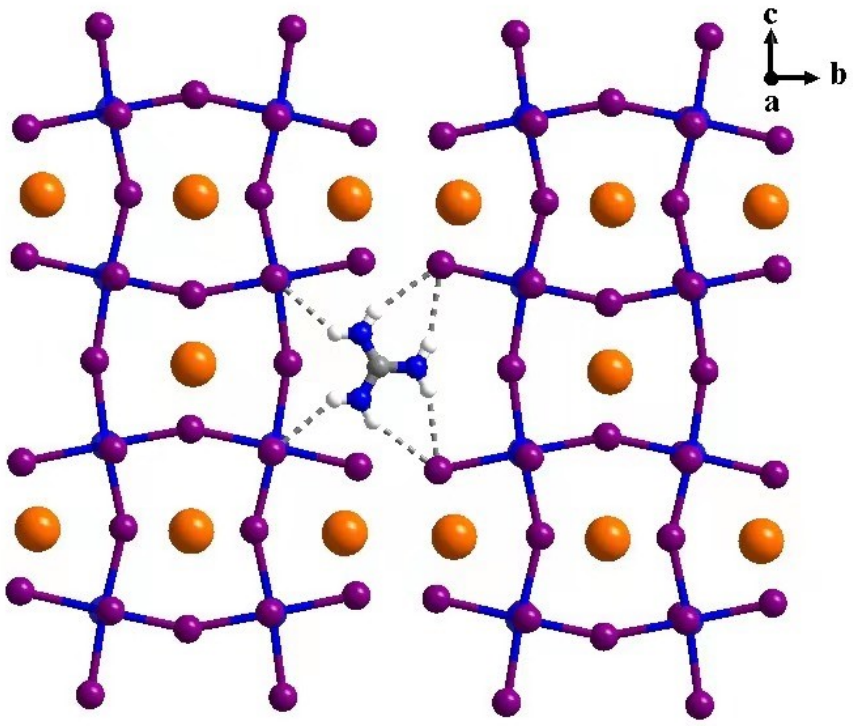

Figure S6. Hydrogen bonds in the compound $Cs_2[C(NH_2)_3]Pb_2Br_7$

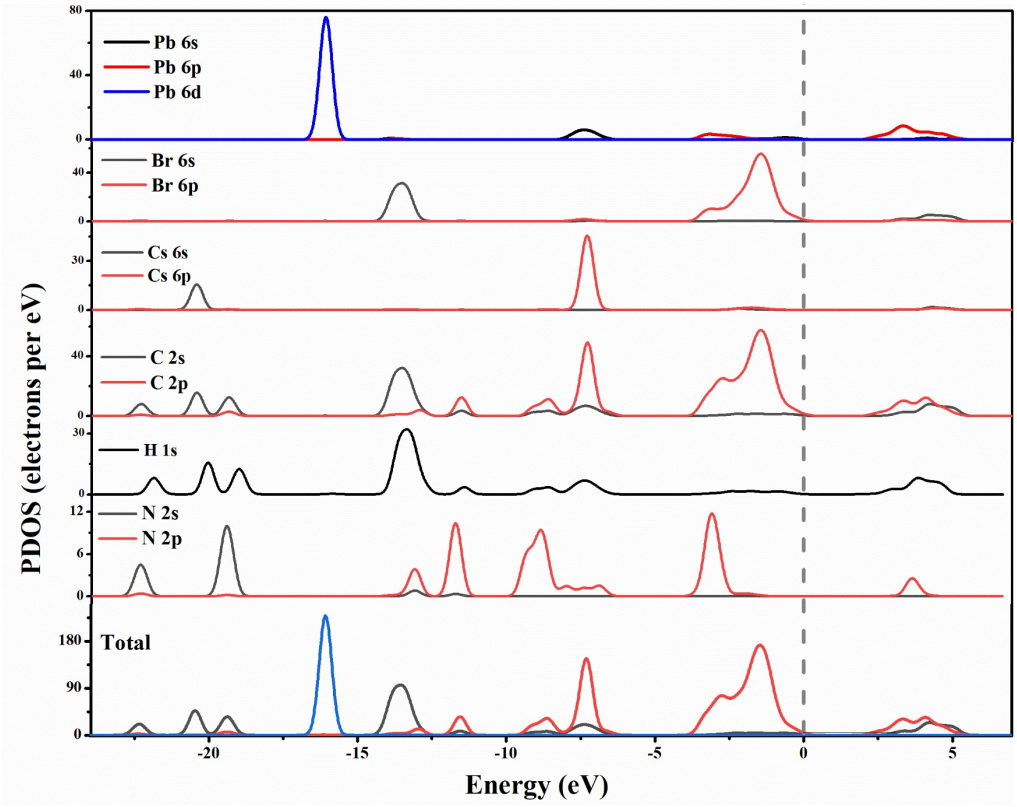

Figure S7. PDOS of the compound $Cs_2[C(NH_2)_3]Pb_2Br_7$

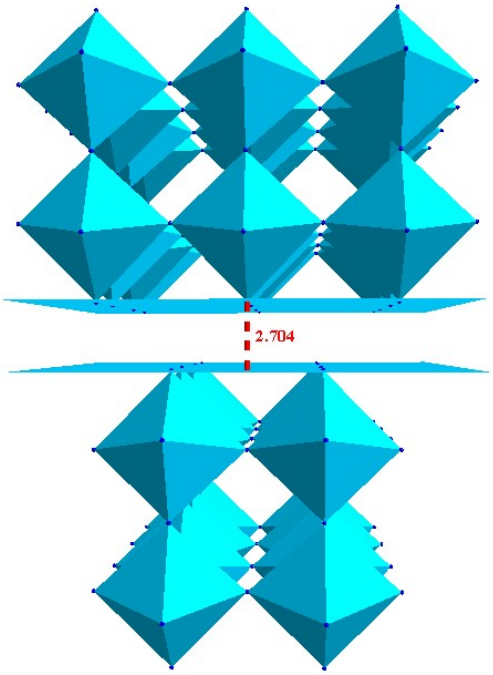

Figure S8. The distance between quantum wells

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Table S1. Crystal Data and Structure Refinement for $Cs_2[C(NH_2)_3]Pb_2Br_7$

Empirical formula	$CH_6Br_7Cs_2N_3Pb_2$
Formula weight	1299.66
Temperature/K	200.00
Space group	Cmmm
a/Å	5.99490(10)
b/Å	28.7131(9)
c/Å	11.5805(3)
α/°	90
β/°	90
γ/°	90
Volume/ Å^3	1993.38(9)
Z	4
ρ_{calc}g/cm^3	4.331
μ/mm^{-1}	34.481
F(000)	2208.0
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.518 to 55.052
Index ranges	$-7 \le h \le 7$, $-37 \le k \le 32$, $-15 \le l \le 14$
Reflections collected	7319

Independent reflections	1332 [Rint = 0.0404, Rsigma = 0.0300]
Data/restraints/parameters	1332/0/55
Goodness-of-fit on F^2	1.259
Final R indexes [I>=2σ (I)]	R1 = 0.0460, wR2 = 0.1167
Largest diff. peak/hole / e $Å^{-3}$	2.05/-5.45

Table S2. The Pb - Br bond lengths of $Cs_2[C(NH_2)_3]Pb_2Br_7$

Bond	(Å)	Bond	(Å)
Pb(1) - Br(5)	2.9759(15)	Pb(1) - Br(8)[1]	3.00339(15)
Pb(1) - Br(6)	2.9477(7)	Pb(1) - Br(8)	3.00339(15)
Pb(1) - Br(7)	2.9795(7)	Pb(1) - Br(9)	2.9465(6)

Table S3. The bond angles of $Cs_2[C(NH_2)_3]Pb_2Br_7$

Bond	Angle/°	Bond	Angle/°
Br(5) - Pb(1) – Br(7)	178.91(6)	Br(9) - Pb(1) – Br(7)	175.53(8)
Br(5) - Pb(1) – Br(8)[1]	92.80(4)	Br(9) - Pb(1) – Br(7)	86.92(8)
Br(5) - Pb(1) – Br(8)	92.80(4)	Br(9) - Pb(1) – Br(7)	92.05(4)
Br(6) - Pb(1) – Br(5)	90.30(6)	Br(9) - Pb(1) – Br(7)	92.05(4)
Br(6) - Pb(1) – Br(7)	88.61(7)	Pb(1) - Br(1) – Pb(7)	154.43(11)
Br(6) - Pb(1) – Br(8)	87.72(4)	Pb(1) - Br(1) – Pb(7)	157.23(11)
Br(6) - Pb(1) – Br(8)[1]	87.72(4)	Pb(1) - Br(1) – Pb(7)	172.79(8)
Br(7) - Pb(1) – Br(8)[1]	87.15(4)	Pb(1)[5] - Br(1) – Pb(7)	163.38(13)
Br(7) - Pb(1) – Br(8)	87.15(4)	N(2) – C00C – N(7)	118.8(11)
Br(8)[1] - Pb(1) – Br(8)	172.79(8)	N(2)[5] – C00C – N(7)	118.8(11)
Br(9) - Pb(1) – Br(5)	94.17(7)	N(2)[5] – C00C – N(7)	122(2)

[1]1+X,+Y,+Z; [2]+X,+Y,1-Z; [3]2-X,1-Y,+Z; [4]-1+X,+Y,+Z; [5]+X,+Y,-Z

Experiment

Synthesis and Crystal Growth: To obtain the single crystal of 1, cesium bromide (CsBr, 5mmol), guanidinium carbonate (G2CO3, 15mmol) and lead(II) bromide (PbBr2, 10mmol) were dissolved in 50mL of aqueous HBr (48% by mass), strong gas evolution was observed, and a yellow precipitate formed. Large-size crystals were grown through temperature cooling method..

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Powder X-Ray Diffraction Analysis: Powder X-Ray Diffractometer (PXRD) patterns were conducted with the MiniFlex II X-ray diffractometer to examine the phase purity of 1. The experimental PXRD patterns were recorded in the 2theta (2θ) range of 5°−50°with a step size of 5°. The experimental PXRD patterns was obtained at room

temperature matching fairly well with the calculated data based on the single-crystal structure, which solidly confirmed the purity of the crystals of 1 (Figure S2).

Crystal Structure Determination: Single-crystal X-ray diffraction was conducted via Bruker D8 Quesr/Venture diffractometer with Mo Kα radiation (λ = 0.77 Å). Crystal structure of Cs2[C(NH2)3]Pb2Br7 was solved through direct method and was refined via the full-matrix least squares refinements on F2 using SHELXLTL software package. Crystal data and structure information are published in Tables S1−S3, Supporting Information.

Ultraviolet-visible (UV−vis) Absorption Spectrum: UV−vis diffuse reflectance spectroscopies of desired materials were performed at room temperature on Perkin-Elmer Lambda 950 UV−vis−IR spectrophotometer in a variable wavelength range between 300 to 700 nm. The BaSO4 was used as the 100 % reflectance reference, and the powdered crystals were used for the measurements. Near the cut-off of the optical transmission, the band gap, the absorption and the wave frequency obey the equation:

$\alpha hv = A(hv - Eg)\ n/2$

Where α, v, A, and Eg are absorption coefficient, light frequency, proportionality constant, and band gap, respectively.

[CCDC 2115841 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.]