Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

(γ-Methoxy propyl amine)$_2$PbBr$_4$: A Novel Two-dimensional Halide Hybrid Perovskite with Efficient Bluish White-light Emission

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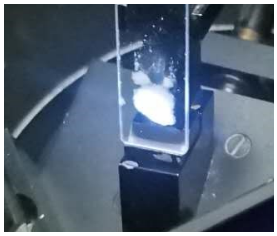

Figure S1. The photo-image of the ***γ*-MPAPB** microscale crystals under UV (365 nm) irradiation.

Figure S2. The bulk single crystal and microscale crystals of ***γ*-MPAPB**.

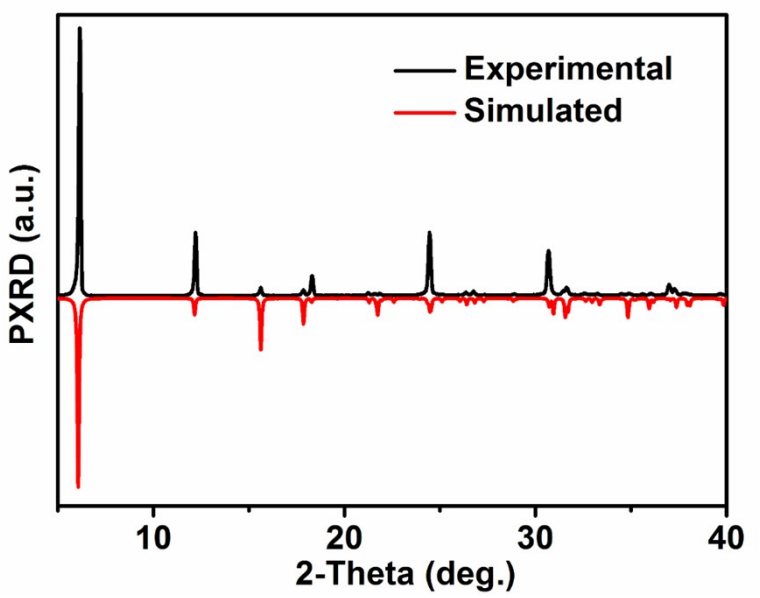

Figure S3. Simulated (black) and experimental (red) PXRD patterns of ***γ*-MPAPB**.

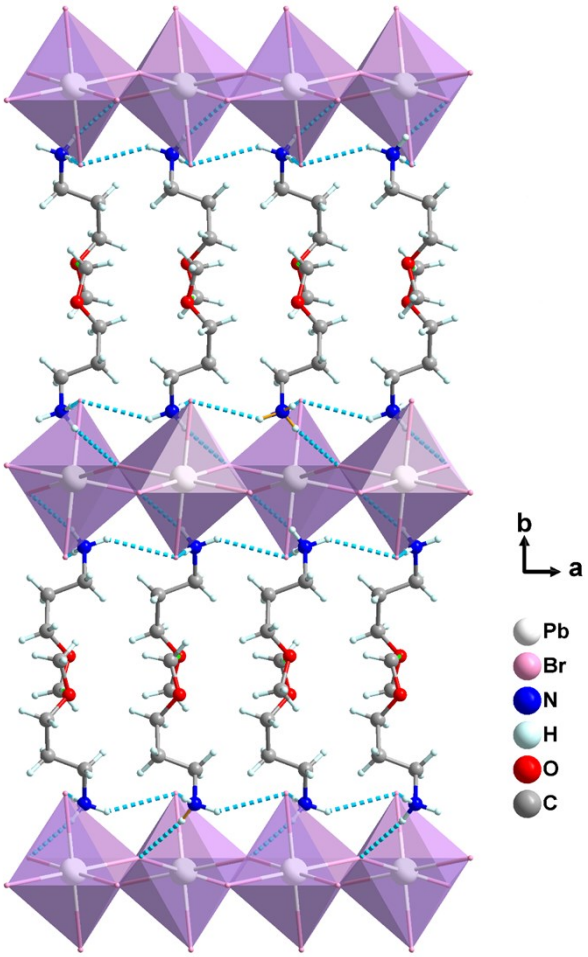

Figure S4. The packing framework of ***γ*-MPAPB** at ab plane.

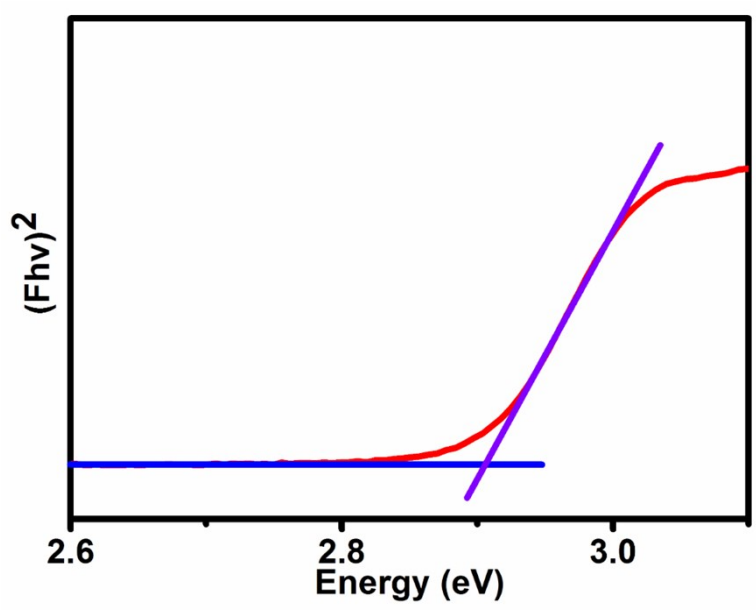

Figure S5. Band gap obtained from optical absorption spectrum of ***γ*-MPAPB**.

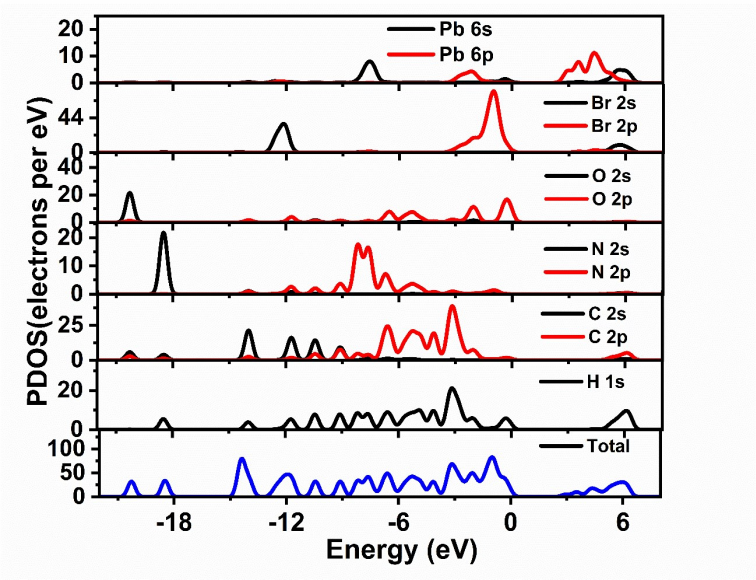

Figure S6. PDOS spectra of ***γ*-MPAPB**.

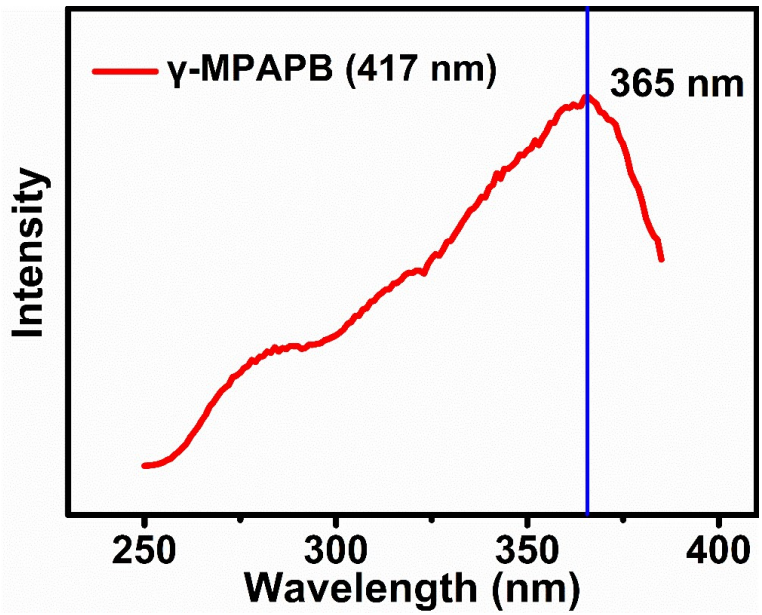

Figure S7. Excitation spectrum of ***γ*-MPAPB**.

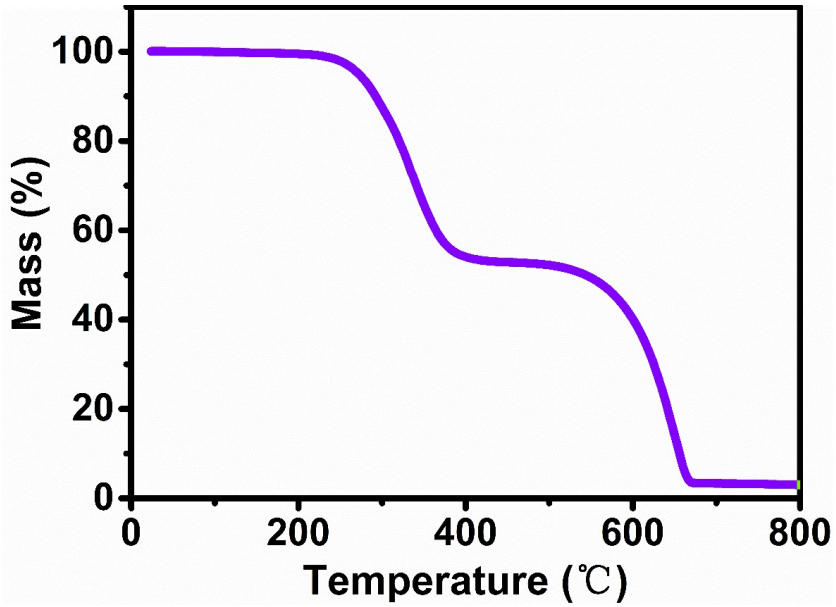

Figure S8. TG curve of compound ***γ*-MPAPB.**

Table S1. Crystal data for ***γ*-MPAPB** collected at 272 K.

Temperature/K	272
Empirical formula	$C_8H_{24}Br_4N_2O_2Pb$
Crystal system	orthorhombic, *Pbca*
Cell parameters	a = 8.1685(10) Å b = 29.085(5) Å c = 8.169 Å
V (Å^3)	1940.7(4)
Z, ρcal. (g/cm^3)	4, 2.420
F(000)	1296.0
Theta range (°)	5.602 to 49.986
Limiting indices	-9 ≤ h ≤ 9, -34 ≤ k ≤ 34, -9 ≤ l ≤ 9
Reflections collected / unique	9366, 1703 [Rint = 0.1790, Rsigma = 0.1000]
Data/restraints/parameter	1703/8/81
Completeness	100
GOF	1.053
Final R indices [I > 2σ(I)]	R1 = 0.0656, wR2 = 0.1537
R indices (all data)	R1 = 0.0917, wR2 = 0.1754
Largest diff. peak and hole	1.36, -2.94 e.A^{-3}

Table S2. Hydrogen lengths and angles of ***γ*-MPAPB** at 272 K.

Bond	D...A (Å)	D - H...A (°)
N(1)—H(1A)···Br(2)	3.430	167.1
N(1)—H(1B)···Br(1)	3.345	159.8
N(1)—H(1C)···Br(1)	3.426	146.7
C(4)—H(4B)···O(1)	3.60	175.1

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

Table S3. Bond Lengths of ***γ*-MPAPB.**

Atom Atom	Length/Å	Atom Atom	Length/Å
Pb1 Br2[1]	2.9861(13)	N1 C1	1.535(16)
Pb1 Br2	2.9913(13)	O1 C3	1.377(15)
Pb1 Br2[2]	2.9861(13)	O1 C4	1.400(14)
Pb1 Br2[3]	2.9914(13)	C3 C2	1.589(17)
Pb1 Br1	2.9672(17)	C1 C2	1.477(18)
Pb1 Br1[3]	2.9672(17)		

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

Table S4. Bond Angles of ***γ*-MPAPB.**

Atom Atom Atom	Angle/˚	Atom Atom Atom	Angle/˚
Br2[1] Pb1 Br2[2]	180.00(7)	Br1 Pb1 Br2[2]	93.14(5)
Br2 Pb1 Br2[3]	180.0	Br1 Pb1 Br2[1]	86.86(5)
Br2[2] Pb1 Br2[3]	88.337(15)	Br1 Pb1 Br2[3]	88.83(5)
Br2[1] Pb1 Br2	88.337(15)	Br1[3] Pb1 Br2	93.14(5)
Br2[1] Pb1 Br2[3]	91.663(15)	Br1 Pb1 Br1[3]	180.0
Br2[2] Pb1 Br2	91.663(15)	Pb1[4] Br2 Pb1	150.17(6)
Br1 Pb1 Br2	91.17(5)	C3 O1 C4	108.1(14)
Br1[3] Pb1 Br2[3]	91.17(5)	O1 C3 C2	108.2(16)
Br1[3] Pb1 Br2[2]	86.86(5)	C2 C1 N1	101.2(13)
Br1[3] Pb1 Br2	88.83(5)	C1 C2 C3	104.0(15)

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