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

Designing Guanidine-based Lead-free hybrid indium perovskites with highly efficient intrinsic broadband emissions

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Table S1. Crystal data and structure refinement for $(C_{13}H_{14}N_3)_3InBr_6$ single crystal.

Compound	$(C_{13}H_{14}N_3)_3InBr_6$
Chemical formula	$C_{39}H_{42}Br_6N_9In$
Formula weight	1239.09
Temperature/K	220
Crystal system	Trigonal
Space group	R3
a/Å	16.492(2)
b/Å	16.492(2)
c/Å	14.152(4)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	3333.6(13)
Z	3
ρ_{calc}g/cm^3	1.840
μ/mm^{-1}	5.965
F(000)	1794
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.39 to 55.066
Index ranges	-19<=h<=21, -21<=k<=21, -18<=l<=18
Reflections collected	26582
Independent reflections	3408 [R(int) = 0.1134, R_{sigma} = 0.0631]
Data/restraints/parameters	3408 / 12 / 67
Goodness-of-fit on F^2	1.049
Final R indexes [I>=2σ (I)]	R1 = 0.0723, wR2 = 0.1862
Final R indexes [all data]	R1 = 0.1494, wR2 = 0.2697
Largest diff. peak/hole / e.Å^{-3}	1.58/-1.36
Flack parameter	0.51(2)

Table S2. Selected Bond lengths (Å) and angles (°) for $(C_{13}H_{14}N_3)_3InBr_6$.

Bond	Distance
In00-Br1^1	2.671(4)
In00-Br1^2	2.670(4)
In00-Br1	2.671(4)
In00-Br	2.687(4)
In00-Br^1	2.687(4)
In00-Br^2	2.687(4)
Angle	(°)
Br1^1-In00-Br1^2	92.08(17)
Br1^1-In00-Br1	92.08(17)
Br1^2-In00-Br1	92.08(17)
Br1^2-In00-Br^1	179.5(2)
Br1-In00-Br^1	88.33(11)

$Br1^2$-In00-Br^2	88.11(11)
$Br1^2$-In00-Br	88.33(11)
$Br1^1$-In00-Br^1	88.11(11)
Br1-In00-Br^2	179.5(2)
Br1-In00-Br	88.11(11)
$Br1^1$-In00-Br	179.5(2)
$Br1^1$-In00-Br^2	88.33(11)
Br^2-In00-Br	91.48(16)
Br^1-In00-Br	91.48(16)
Br^2-In00-Br^1	92.08(17)

Table S3. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for $(C_{13}H_{14}N_3)_3InBr_6$.

Atom	x	y	z	$U_{(eq)}$
In00	6666.67	3333.33	6735(4)	50.4(6)
Br1	7302(2)	4879(2)	7784.4(14)	56.6(11)
Br	5759(2)	3974(2)	5667.7(12)	54.8(10)
C005	8380(20)	6758(19)	5070(20)	70(7)
N006	9296(15)	7542(15)	5349(13)	71(4)
C007	6825(14)	6453(10)	3312(15)	80(2)
C00D	7380(13)	6145(12)	3744(15)	80(2)
C00G	7207(14)	5240(13)	3583(17)	80(2)
C009	6479(15)	4644(10)	2990(17)	80(2)
C00K	5924(13)	4952(12)	2558(15)	80(2)
C00A	6098(13)	5856(13)	2719(15)	80(2)
C008	9929(16)	7036(11)	6651(15)	80(2)
C00B	9623(14)	7629(13)	6316(13)	80(2)
C00H	9906(15)	8481(12)	6762(15)	80(2)
C00J	10494(15)	8738(11)	7543(15)	80(2)
C00E	10800(13)	8144(13)	7878(13)	80(2)
C00C	10518(15)	7293(12)	7432(15)	80(2)
N1	8287(15)	6863(14)	4146(15)	71(4)
N2	7926(14)	6098(15)	5646(14)	71(4)

Table S4. Anisotropic displacement parameters (Å^2 × 10^3) for $(C_{13}H_{14}N_3)_3InBr_6$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
In00	54.2(8)	54.2(8)	43.0(11)	0	0	27.1(4)
Br1	62(2)	61(2)	49(2)	-5.7(18)	3.4(18)	33(2)
Br	62(2)	59(2)	45(2)	-2.2(17)	-8.8(16)	31(2)
C005	99(17)	95(19)	65(13)	-35(13)	-26(12)	85(16)
N006	76(10)	60(9)	71(9)	25(7)	23(7)	29(7)
C007	76(5)	63(5)	108(6)	-9(5)	-29(4)	39(4)

C00D	76(5)	63(5)	108(6)	-9(5)	-29(4)	39(4)
C00G	76(5)	63(5)	108(6)	-9(5)	-29(4)	39(4)
C009	76(5)	63(5)	108(6)	-9(5)	-29(4)	39(4)
C00K	76(5)	63(5)	108(6)	-9(5)	-29(4)	39(4)
C00A	76(5)	63(5)	108(6)	-9(5)	-29(4)	39(4)
C008	76(5)	63(5)	108(6)	-9(5)	-29(4)	39(4)
C00B	76(5)	63(5)	108(6)	-9(5)	-29(4)	39(4)
C00H	76(5)	63(5)	108(6)	-9(5)	-29(4)	39(4)
C00J	76(5)	63(5)	108(6)	-9(5)	-29(4)	39(4)
C00E	76(5)	63(5)	108(6)	-9(5)	-29(4)	39(4)
C00C	76(5)	63(5)	108(6)	-9(5)	-29(4)	39(4)
N1	76(10)	60(9)	71(9)	25(7)	23(7)	29(7)
N2	76(10)	60(9)	71(9)	25(7)	23(7)	29(7)

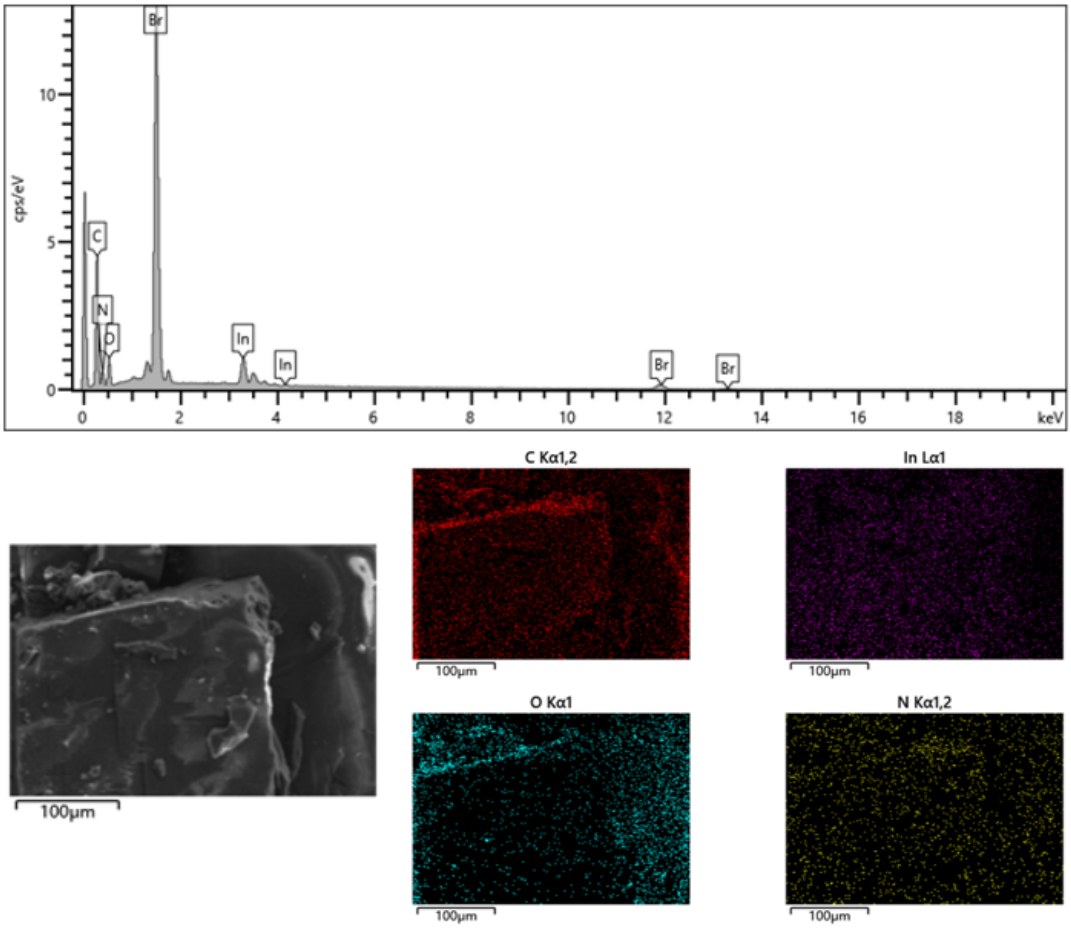

Figure S1. EDS spectrum of $(C_{13}H_{14}N_3)_3InBr_6$.

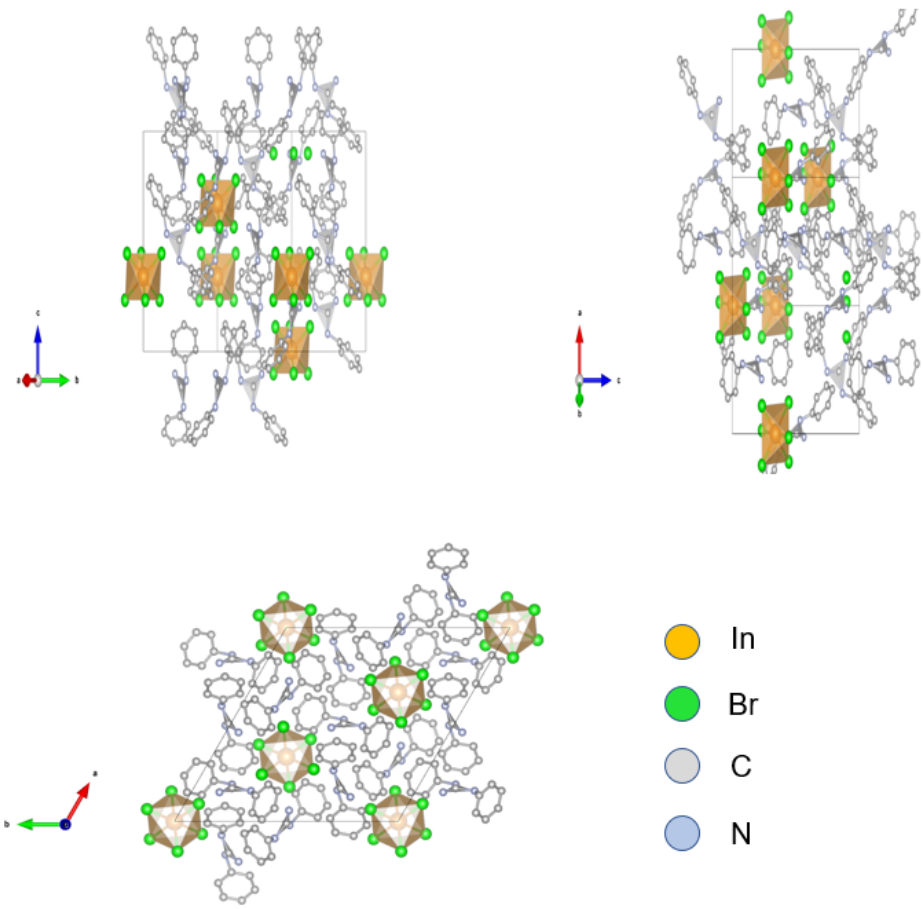

Figure S2. Single crystal structure of 0D $(C_{13}H_{14}N_3)_3InBr_6$ from different viewing directions (brown, green, grey, blue spheres represent In, Br, C and N atoms, respectively).

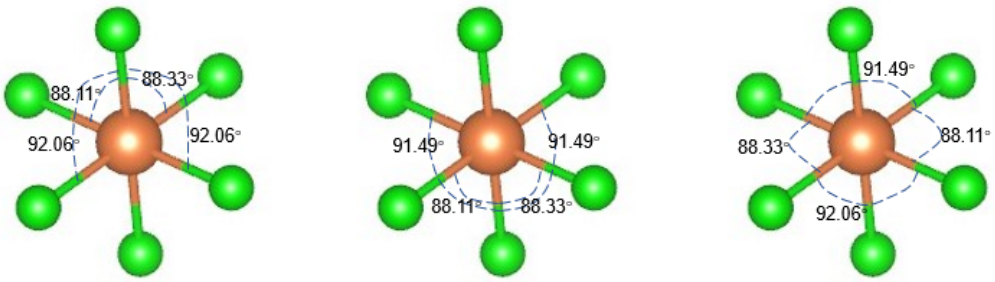

Figure S3. Bond angles of $[InBr_6]^{3-}$ octahedron anion in $(C_{13}H_{14}N_3)_3InBr_6$.

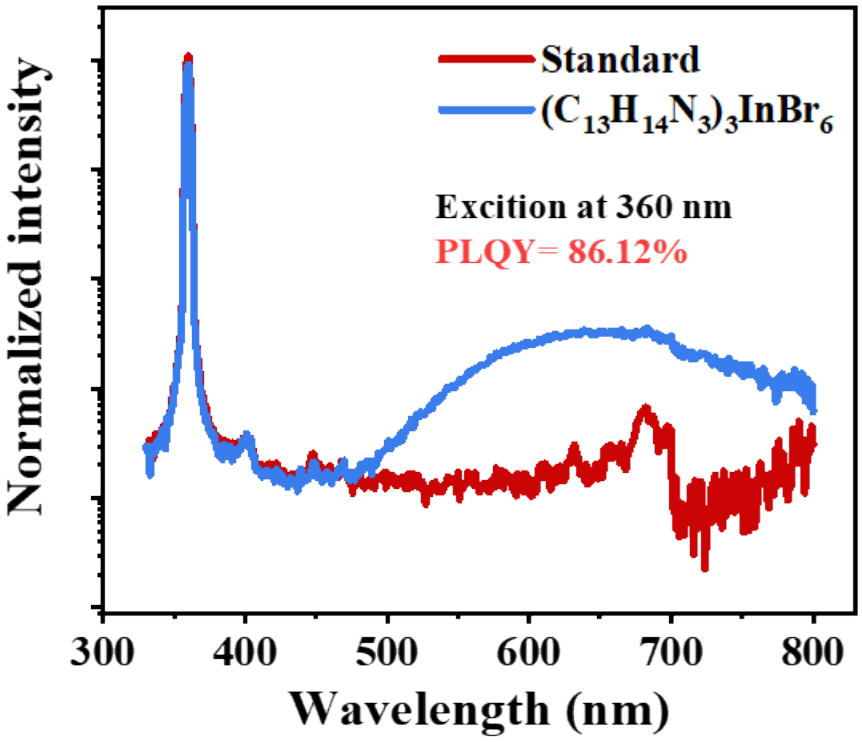

Figure S4. The PLQE curves of $(C_{13}H_{14}N_3)_3InBr_6$.

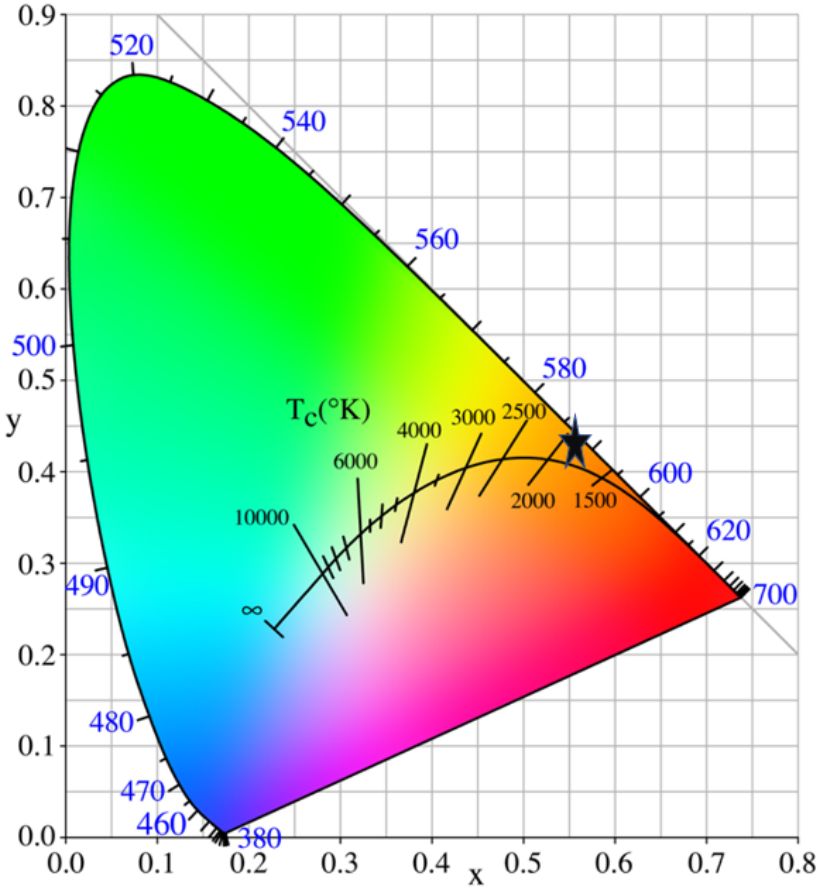

Figure S5. CIE chromaticity coordinates of $(C_{13}H_{14}N_3)_3InBr_6$ single crystals (black star).

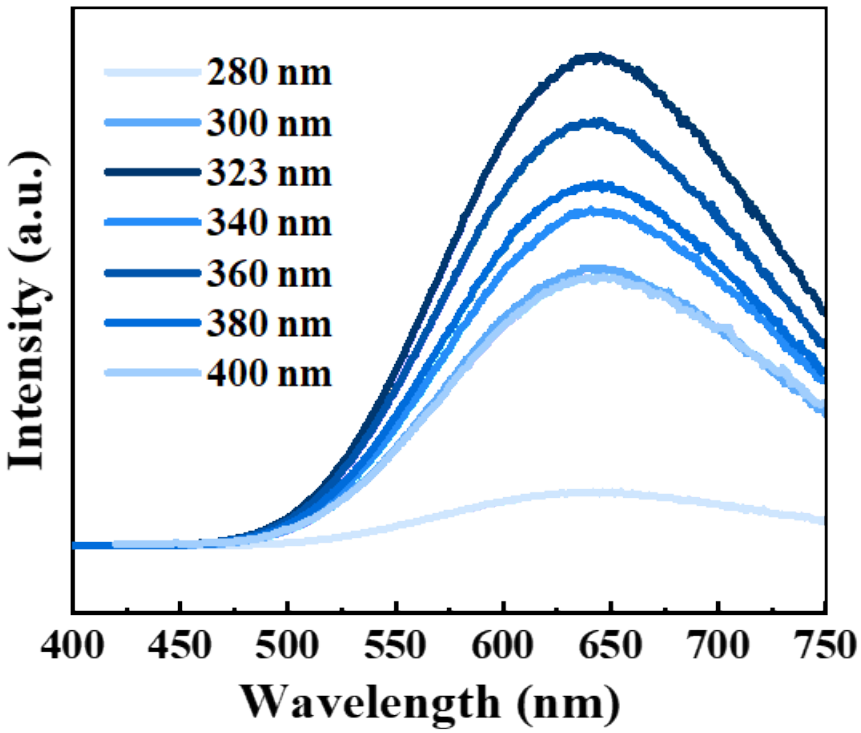

Figure S6. PL collected across the broadband emission for $(C_{13}H_{14}N_3)_3InBr_6$.

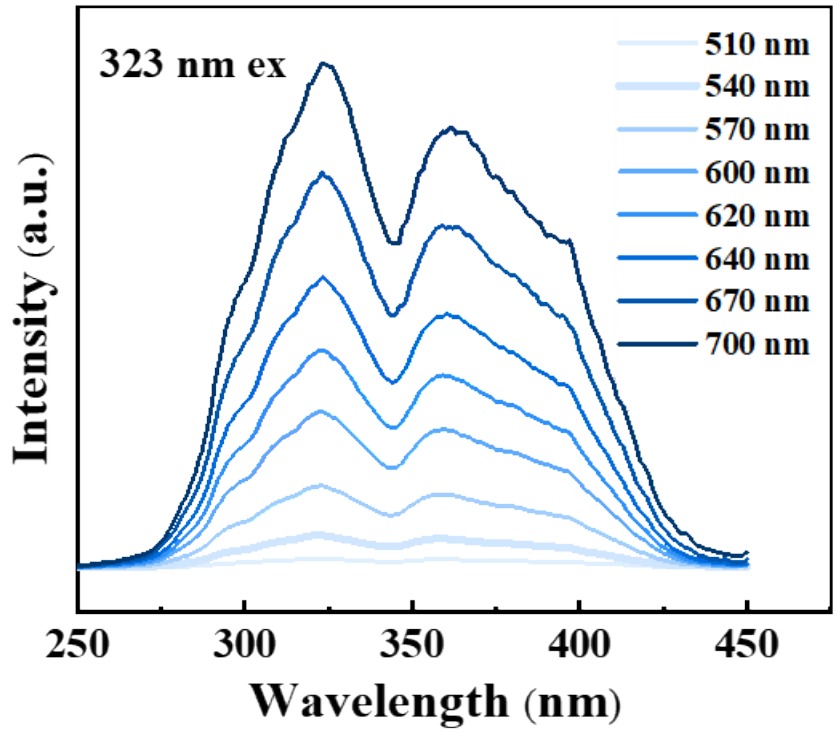

Figure S7. PLE collected across the broadband emission for $(C_{13}H_{14}N_3)_3InBr_6$.

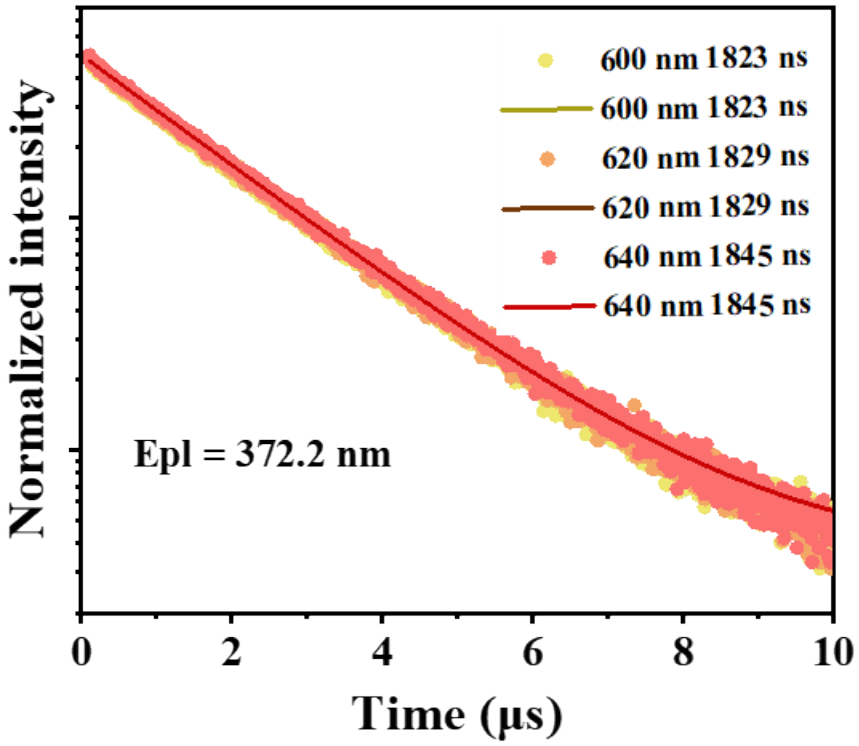

Figure S8. Time-resolved PL decay curves of $(C_{13}H_{14}N_3)_3InBr_6$ collected across the broadband emission at room temperature.

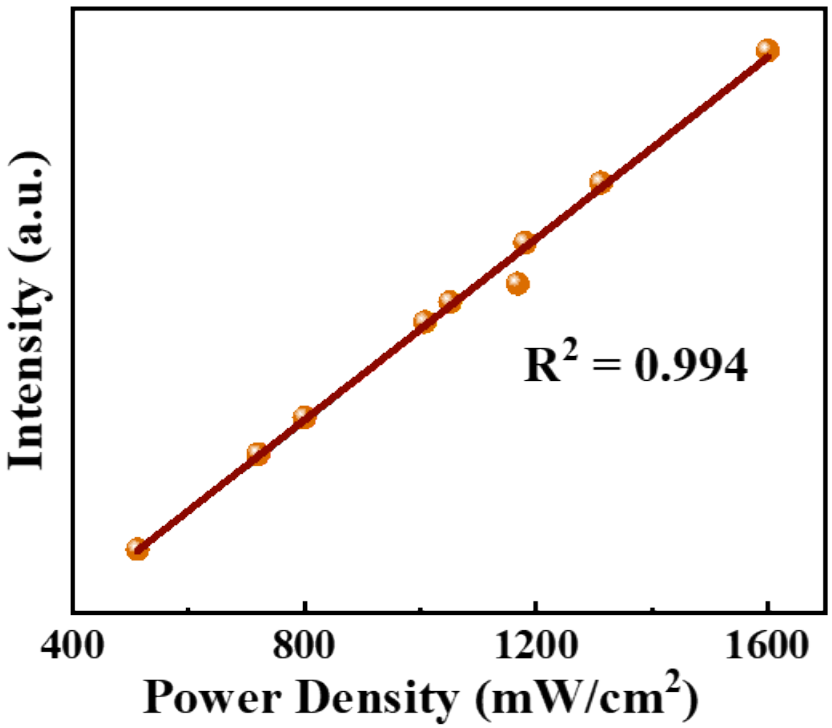

Figure S9. Excitation power density dependent PL emission intensity of $(C_{13}H_{14}N_3)_3InBr_6$.

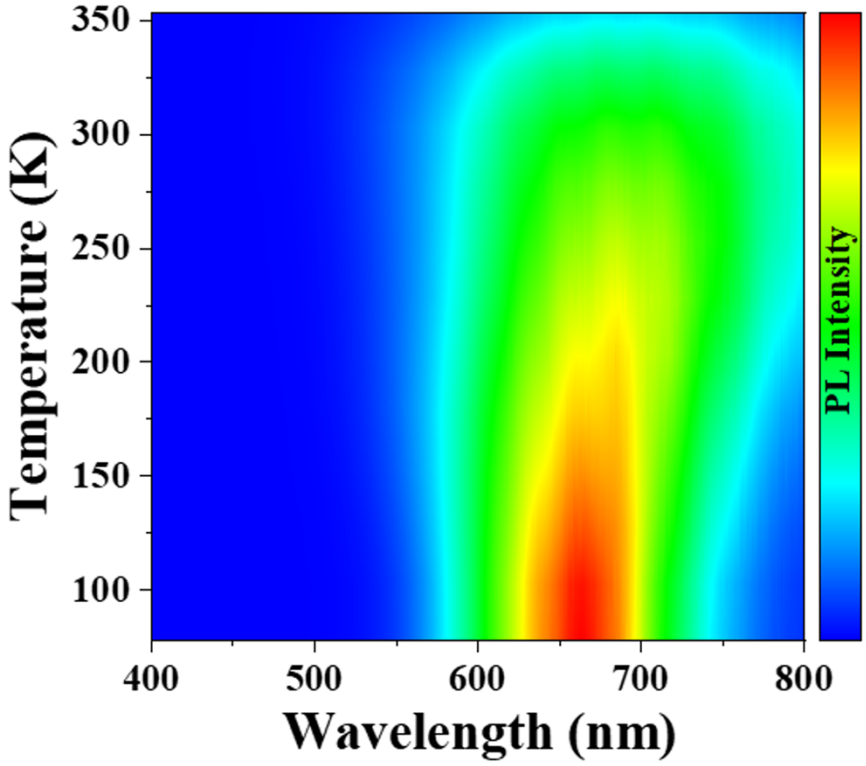

Figure S10. Temperature-dependent steady-state emission spectra of $(C_{13}H_{14}N_3)_3InBr_6$ crystals excited by 360 nm (78-353 K).

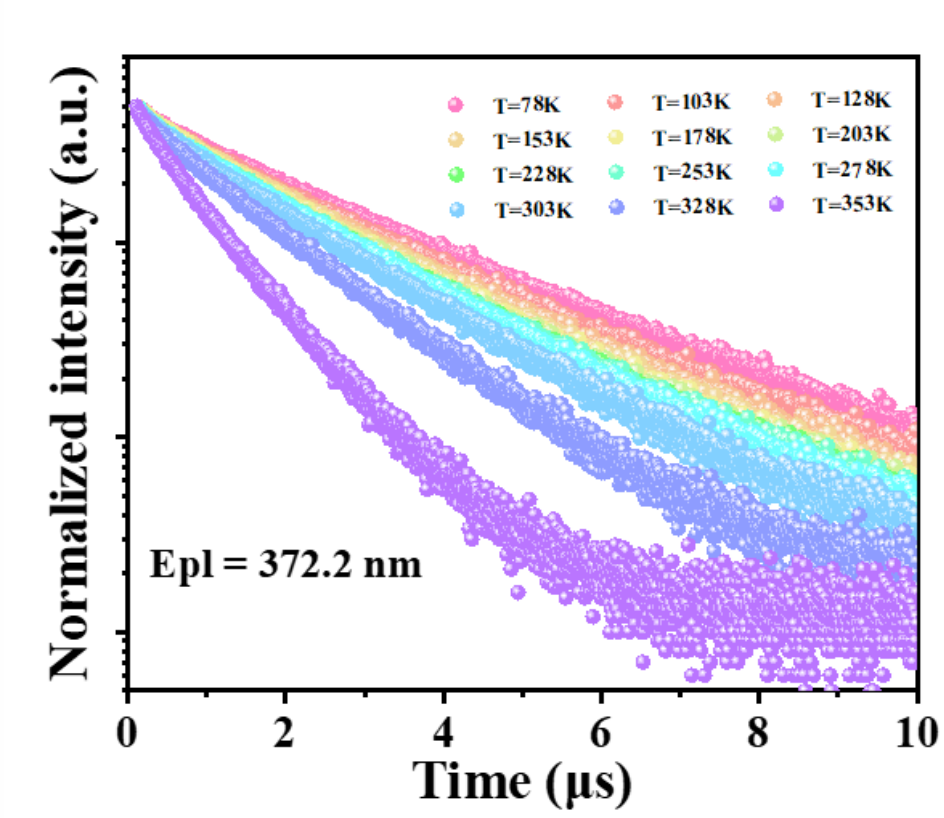

Figure S11. Temperature-dependent time-resolved PL decay curves of $(C_{13}H_{14}N_3)_3InBr_6$ crystals excited by 372.2 nm (78-353 K)