Supporting Information for:

High Efficiency Red Photoluminescence Achieved by Antimony Doping in Organic-Inorganic Hybrid Halide $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$

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Table S1. Crystal data and structure refinement of $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$ at 300 K.

Empirical formula	$(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$
Formula weight	1397.38
Temperature	300 K
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group	*Pbca*
Unit cell dimensions	a = 15.7695(17) Å, α = 90°
	b = 15.8071(15) Å, β = 90°
	c = 31.957(13) Å, γ = 90°
Volume	7965.8(15) Å^3
Z	8
Density (calculated)	2.330 g/cm^3
Absorption coefficient	11.210 mm^{-1}
F(000)	5248
Crystal size	0.18 × 0.15 ×0.08 mm^3
θ range for data collection	2.225 to 26.458°
Index ranges	-19 ⩽ h ⩽ 19
	-19 ⩽ k ⩽ 19
	-40 ⩽ l ⩽ 40
Reflections collected	71812
Independent reflections	8175 [R_{int} = 0.0948]
Completeness	99.8%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8175/0/343
Goodness-of-fit	1.014
Final R indices [$I > 2\sigma(I)$]	R_{obs} = 0.0558, wR_{obs} = 0.1363
R indices [all data]	R_{all} = 0.1015, wR_{all} = 0.1628
Largest diff. peak and hole	0.949 and -1.076 e·Å^{-3}

$R = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2]/\Sigma[w(|F_o|^4)]\}^{1/2}$ and $w = 1/[\sigma^2(F_o^2) + (0.0795P)^2 + 25.4742P]$ where $P = (F_o^2 + 2F_c^2)/3$

Table S2. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$ at 300 K with estimated standard deviations in parentheses.

Label	*x*	*y*	*z*	Occupancy	U_{eq}*
In(1)	3682(1)	7816(1)	4812(1)	1	49(1)
In(2)	3662(1)	4914(1)	7004(1)	1	67(1)
Br(3)	2320(1)	7068(1)	4466(1)	1	54(1)
Br(5)	2549(1)	8676(1)	5278(1)	1	56(1)
Br(4)	3683(1)	6505(1)	5346(1)	1	56(1)
Br(2)	4880(1)	6872(1)	4401(1)	1	56(1)
Br(6)	4955(1)	8493(1)	5230(1)	1	58(1)
Br(1)	3677(1)	8975(1)	4222(1)	1	66(1)
Br(8)	4962(1)	5565(1)	7304(1)	1	80(1)
Br(9)	3506(1)	3390(1)	7165(1)	1	85(1)
Br(7)	3750(2)	5045(2)	6225(1)	1	118(1)
Br(10)	2382(1)	5727(2)	7216(1)	1	134(1)
N(2)	6151(5)	9382(4)	3824(3)	1	51(2)
N(3)	5833(4)	6340(4)	5425(3)	1	52(2)
N(1)	6569(5)	8270(5)	4506(3)	1	57(2)
N(4)	6237(5)	5196(5)	6112(3)	1	59(2)
C(2)	6117(6)	8441(5)	3774(3)	1	54(2)
C(5)	5542(6)	9797(6)	3521(3)	1	58(3)
C(3)	5976(5)	9633(6)	4259(3)	1	50(2)
C(1)	6736(6)	8024(6)	4071(3)	1	57(2)
C(17)	6691(6)	3860(6)	6483(3)	1	57(2)
C(6)	5527(6)	10758(6)	3549(3)	1	55(2)
C(15)	6236(6)	6149(6)	6159(3)	1	60(3)
C(11)	4953(7)	11085(6)	3203(4)	1	70(3)
C(14)	6468(6)	5003(6)	5661(4)	1	59(3)
C(12)	5857(6)	5415(6)	5362(3)	1	56(2)

C(16)	6842(7)	4803(7)	6408(4)	1	76(3)
C(7)	6405(7)	11136(6)	3504(4)	1	73(3)
C(13)	5627(6)	6564(6)	5861(3)	1	57(2)
C(4)	6603(6)	9206(6)	4558(4)	1	62(3)
C(18)	5895(7)	3654(7)	6731(4)	1	78(3)
C(10)	4889(10)	12062(7)	3222(5)	1	96(4)
C(20)	6562(9)	2345(9)	7029(5)	1	101(5)
C(8)	6350(8)	12103(6)	3537(5)	1	85(4)
C(9)	5729(10)	12464(8)	3218(5)	1	104(5)
C(22)	7469(7)	3499(8)	6721(5)	1	88(4)
C(21)	7347(8)	2545(7)	6790(4)	1	83(4)
C(19)	5807(8)	2705(8)	6789(5)	1	95(4)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S3. Anisotropic displacement parameters (Å^2 × 10^3) for $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$ at 300 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
In(1)	40(1)	52(1)	57(1)	1(1)	1(1)	6(1)
In(2)	67(1)	67(1)	66(1)	4(1)	-9(1)	7(1)
Br(3)	45(1)	59(1)	57(1)	-1(1)	-2(1)	-3(1)
Br(5)	50(1)	53(1)	65(1)	2(1)	5(1)	-4(1)
Br(4)	44(1)	60(1)	66(1)	1(1)	1(1)	16(1)
Br(2)	47(1)	58(1)	64(1)	0(1)	8(1)	-3(1)
Br(6)	47(1)	64(1)	63(1)	-4(1)	1(1)	-6(1)
Br(1)	50(1)	72(1)	76(1)	1(1)	4(1)	24(1)
Br(8)	76(1)	72(1)	94(1)	1(1)	-22(1)	8(1)
Br(9)	89(1)	75(1)	90(1)	-2(1)	6(1)	20(1)
Br(7)	162(2)	126(2)	66(1)	-43(2)	-24(1)	34(1)
Br(10)	71(1)	120(2)	211(2)	24(1)	-32(1)	-74(2)
N(2)	54(4)	47(4)	51(5)	0(3)	5(4)	3(4)

N(3)	43(4)	56(4)	56(6)	0(3)	-2(4)	7(4)
N(1)	42(4)	57(4)	72(6)	-1(3)	4(4)	22(4)
N(4)	55(4)	64(5)	58(6)	-9(4)	-7(4)	7(4)
C(2)	61(5)	50(5)	50(6)	0(4)	2(5)	-3(4)
C(5)	56(5)	54(5)	63(7)	-5(4)	-5(5)	5(5)
C(3)	48(5)	55(5)	48(6)	-1(4)	5(4)	-2(4)
C(1)	59(6)	51(5)	61(7)	4(4)	5(5)	9(5)
C(17)	59(5)	63(6)	50(7)	7(5)	2(5)	1(5)
C(6)	59(5)	57(5)	50(6)	15(4)	-11(5)	-4(5)
C(15)	69(6)	54(5)	56(7)	-1(5)	-4(5)	-12(5)
C(11)	77(7)	66(6)	68(8)	23(5)	-18(6)	-5(6)
C(14)	48(5)	50(5)	80(8)	0(4)	-8(5)	-6(5)
C(12)	58(5)	50(5)	62(7)	-6(4)	-2(5)	-4(5)
C(16)	75(7)	85(7)	68(8)	-9(6)	-20(6)	21(6)
C(7)	74(7)	65(6)	79(9)	-2(5)	2(6)	9(6)
C(13)	57(5)	51(5)	63(7)	1(4)	1(5)	5(5)
C(4)	47(5)	63(6)	75(8)	-9(4)	-7(5)	9(5)
C(18)	71(7)	87(8)	76(9)	26(6)	26(6)	20(6)
C(10)	134(12)	71(7)	83(10)	27(8)	-39(9)	7(7)
C(20)	106(10)	102(10)	95(12)	14(8)	15(9)	40(8)
C(8)	108(10)	53(6)	94(10)	-11(6)	-6(8)	9(6)
C(9)	158(14)	58(7)	97(12)	-6(8)	-25(10)	22(7)
C(22)	63(6)	95(8)	106(11)	5(6)	-13(7)	26(8)
C(21)	85(8)	92(8)	72(9)	33(7)	-14(7)	9(7)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S4. Crystal data and structure refinement of $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$:$x$Sb^{3+} ($x$ = 0, 0.05 and 0.10) at 150 K.

Empirical formula	$(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$	$(C_{11}H_{24}N_2)_2[In_{0.9}Sb_{0.1}Br_6][InBr_4]$	$(C_{11}H_{24}N_2)_2[In_{0.8}Sb_{0.2}Br_6][InBr_4]$
Formula weight	1397.38	1398.07	1398.77
Temperature		150 K	
Wavelength		0.71073 Å	
Crystal system	orthorhombic	orthorhombic	orthorhombic
Space group	*Pbca*	*Pbca*	*Pbca*
Unit cell dimensions	a = 15.6904(5) Å	a = 15.7197(7) Å	a = 15.7544(5) Å
	b = 15.6905(5) Å	b = 15.7070(6) Å	b = 15.6813(5) Å
	c = 31.7718(13) Å	c = 31.7425(14) Å	c = 31.7067(11) Å
Volume	7821.9(5) Å^3	7837.5(6) Å^3	7833.1(4) Å^3
Z	8	8	8
Density (calculated)	2.373 g/cm^3	2.370 g/cm^3	2.369 g/cm^3
Absorption coefficient	11.416 mm^{-1}	11.404 mm^{-1}	11.420 mm^{-1}
F(000)	5248	5250	5235
θ range for data collection	1.944 to 26.476°	2.237 to 26.399°	2.238 to 26.403°
Index ranges	$-19 \le h \le 19$	$-19 \le h \le 19$	$-15 \le h \le 19$
	$-19 \le k \le 19$	$-19 \le k \le 19$	$-19 \le k \le 19$
	$-39 \le l \le 39$	$-39 \le l \le 39$	$-39 \le l \le 39$
Reflections collected	104432	74336	80310
Independent reflections	8050 [R_{int} = 0.0692]	8015 [R_{int} = 0.1037]	8019 [R_{int} = 0.0945]
Completeness	99.8%	99.9%	99.8%
Refinement method		Full-matrix least squares on F^2	
Data/restraints/parameters	8050/0/343	8015/0/343	8019/0/343
Goodness-of-fit	1.032	1.026	1.020
Final R indices [$I > 2\sigma(I)$]	R_{obs} = 0.0346	R_{obs} = 0.0464	R_{obs} = 0.0466
	wR_{obs} = 0.0786	wR_{obs} = 0.0847	wR_{obs} = 0.1087
R indices [all data]	R_{all} = 0.0480	R_{all} = 0.0789	R_{all} = 0.0724
	wR_{all} = 0.0843	wR_{all} = 0.0945	wR_{all} = 0.1231
Largest diff. peak and hole	0.898 and -0.819 e·Å^{-3}	0.654 and -0.663 e·Å^{-3}	1.039 and -0.794 e·Å^{-3}

Table S5. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$ at 150 K with estimated standard deviations in parentheses.

Label	*x*	*y*	*z*	Occupancy	U_{eq}*
In(1)	3669(1)	2809(1)	4796(1)	1	29(1)
In(2)	6338(1)	10097(1)	2994(1)	1	38(1)
Br(4)	2535(1)	3672(1)	5269(1)	1	32(1)
Br(6)	3672(1)	1489(1)	5331(1)	1	32(1)
Br(5)	2295(1)	2059(1)	4450(1)	1	31(1)
Br(2)	4944(1)	3491(1)	5225(1)	1	33(1)
Br(1)	4885(1)	1873(1)	4386(1)	1	32(1)
Br(3)	3665(1)	3975(1)	4202(1)	1	36(1)
Br(8)	5027(1)	9439(1)	2690(1)	1	42(1)
Br(9)	6514(1)	11631(1)	2833(1)	1	44(1)
Br(10)	6249(1)	9965(1)	3783(1)	1	64(1)
Br(7)	7631(1)	9271(1)	2784(1)	1	76(1)
N(4)	6148(2)	4393(2)	3815(2)	1	30(1)
N(1)	5813(2)	1344(2)	5419(2)	1	30(1)
N(2)	6205(3)	204(3)	6115(2)	1	33(1)
N(3)	6560(3)	3287(3)	4514(2)	1	33(1)
C(16)	5537(3)	4790(3)	3505(2)	1	34(2)
C(12)	6588(3)	4235(3)	4561(2)	1	34(2)
C(14)	5969(3)	4650(3)	4262(2)	1	30(1)
C(3)	5841(3)	400(3)	5363(2)	1	33(2)
C(18)	4946(4)	6104(3)	3186(2)	1	37(2)
C(15)	6124(3)	3441(3)	3774(2)	1	36(2)
C(5)	6808(3)	-198(3)	6434(2)	1	39(2)
C(2)	6198(3)	1150(3)	6169(2)	1	36(2)
C(17)	5513(3)	5762(3)	3538(2)	1	32(2)
C(21)	6320(4)	7134(3)	3554(2)	1	46(2)

C(1)	5597(3)	1574(3)	5862(2)	1	34(2)
C(6)	6676(3)	-1151(3)	6490(2)	1	35(2)
C(4)	6456(3)	0(3)	5667(2)	1	32(2)
C(13)	6746(3)	3024(3)	4076(2)	1	35(2)
C(20)	5707(4)	7507(4)	3234(2)	1	52(2)
C(22)	6396(3)	6168(3)	3512(2)	1	39(2)
C(7)	5861(3)	-1366(3)	6734(2)	1	41(2)
C(19)	4845(4)	7066(3)	3233(2)	1	48(2)
C(11)	7463(4)	-1519(4)	6712(2)	1	43(2)
C(9)	6566(4)	-2672(4)	7029(2)	1	49(2)
C(8)	5781(4)	-2323(4)	6800(2)	1	50(2)
C(10)	7371(4)	-2467(4)	6788(2)	1	46(2)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S6. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$ at 150 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
In(1)	25(1)	30(1)	33(1)	0(1)	1(1)	3(1)
In(2)	38(1)	38(1)	38(1)	2(1)	-5(1)	3(1)
Br(4)	29(1)	30(1)	36(1)	1(1)	2(1)	-2(1)
Br(6)	26(1)	33(1)	36(1)	0(1)	0(1)	7(1)
Br(5)	27(1)	33(1)	32(1)	0(1)	-1(1)	-2(1)
Br(2)	28(1)	35(1)	36(1)	-2(1)	0(1)	-3(1)
Br(1)	28(1)	32(1)	36(1)	0(1)	4(1)	-2(1)
Br(3)	30(1)	39(1)	41(1)	1(1)	1(1)	10(1)
Br(8)	41(1)	38(1)	47(1)	0(1)	-10(1)	5(1)
Br(9)	46(1)	41(1)	46(1)	-1(1)	3(1)	9(1)
Br(10)	86(1)	66(1)	38(1)	-25(1)	-15(1)	17(1)
Br(7)	40(1)	67(1)	122(1)	14(1)	-21(1)	-44(1)
N(4)	29(2)	27(2)	34(2)	0(2)	3(2)	-1(2)

N(1)	25(2)	30(2)	36(2)	-1(2)	-2(2)	1(2)
N(2)	30(2)	36(2)	33(2)	-4(2)	-1(2)	3(2)
N(3)	27(2)	33(2)	38(2)	-1(2)	-2(2)	6(2)
C(16)	33(3)	41(3)	30(3)	2(2)	-4(2)	3(2)
C(12)	32(3)	33(3)	36(3)	-3(2)	-2(2)	-2(2)
C(14)	28(2)	34(3)	29(3)	4(2)	0(2)	1(2)
C(3)	34(3)	32(3)	34(3)	-4(2)	-4(2)	-1(2)
C(18)	43(3)	33(3)	36(3)	7(2)	-7(2)	-5(2)
C(15)	44(3)	28(2)	37(3)	-3(2)	4(2)	-1(2)
C(5)	37(3)	46(3)	35(3)	1(2)	-8(2)	3(2)
C(2)	38(3)	35(3)	33(3)	-5(2)	-2(2)	-4(2)
C(17)	30(3)	35(3)	29(3)	4(2)	-1(2)	1(2)
C(21)	59(4)	34(3)	45(3)	-5(3)	-6(3)	-3(2)
C(1)	33(3)	32(3)	37(3)	-2(2)	2(2)	0(2)
C(6)	32(3)	39(3)	33(3)	1(2)	1(2)	0(2)
C(4)	31(3)	31(3)	32(3)	1(2)	1(2)	-5(2)
C(13)	34(3)	31(3)	39(3)	0(2)	3(2)	0(2)
C(20)	74(4)	33(3)	49(4)	1(3)	-3(3)	4(3)
C(22)	39(3)	37(3)	41(3)	1(2)	1(2)	4(2)
C(7)	39(3)	43(3)	41(3)	9(2)	7(2)	6(2)
C(19)	67(4)	39(3)	37(3)	18(3)	-16(3)	-6(3)
C(11)	44(3)	47(3)	38(3)	5(3)	-5(2)	1(3)
C(9)	57(4)	41(3)	50(4)	11(3)	9(3)	17(3)
C(8)	39(3)	49(3)	61(4)	1(3)	13(3)	16(3)
C(10)	44(3)	50(3)	43(3)	13(3)	-4(3)	9(3)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S7. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $(C_{11}H_{24}N_2)_2[In_{0.9}Sb_{0.1}Br_6][InBr_4]$ at 150 K with estimated standard deviations in parentheses.

Label	*x*	*y*	*z*	Occupancy	U_{eq}*

In(1)	1331(1)	2817(1)	4791(1)	0.9	31(1)
Sb(1)	1331(1)	2817(1)	4791(1)	0.1	31(1)
In(2)	1354(1)	-106(1)	7008(1)	1	40(1)
Br(4)	1332(1)	1482(1)	5329(1)	1	34(1)
Br(2)	2459(1)	3679(1)	5269(1)	1	34(1)
Br(6)	56(1)	3495(1)	5226(1)	1	35(1)
Br(3)	2727(1)	2063(1)	4447(1)	1	36(1)
Br(5)	94(1)	1859(1)	4385(1)	1	38(1)
Br(1)	1337(1)	4004(1)	4195(1)	1	42(1)
Br(10)	38(1)	548(1)	7308(1)	1	44(1)
Br(9)	1520(1)	-1646(1)	7164(1)	1	46(1)
Br(7)	1287(1)	44(1)	6220(1)	1	70(1)
Br(8)	2640(1)	708(1)	7234(1)	1	82(1)
N(1)	4191(4)	3664(3)	4578(2)	1	32(2)
N(4)	3846(4)	614(4)	6186(2)	1	34(2)
N(3)	3432(4)	1720(4)	5489(2)	1	36(2)
N(2)	3799(4)	4815(4)	3883(2)	1	32(2)
C(15)	3416(5)	776(4)	5438(2)	1	36(2)
C(13)	3860(5)	1556(4)	6225(2)	1	37(2)
C(16)	4459(5)	212(4)	6493(2)	1	35(2)
C(22)	5063(5)	-1103(5)	6806(3)	1	41(2)
C(6)	3336(5)	6165(5)	3510(2)	1	35(2)
C(18)	3617(5)	-1173(5)	6495(3)	1	41(2)
C(14)	4035(4)	359(4)	5736(2)	1	31(2)
C(12)	3246(5)	1976(4)	5927(2)	1	38(2)
C(17)	4491(5)	-760(4)	6460(2)	1	32(2)
C(5)	3196(5)	5209(5)	3570(2)	1	40(2)
C(4)	4163(5)	4607(4)	4644(2)	1	34(2)
C(19)	3695(5)	-2139(5)	6447(3)	1	46(2)
C(1)	4413(5)	3442(5)	4136(2)	1	38(2)

C(2)	3815(5)	3860(4)	3828(2)	1	37(2)
C(11)	4139(5)	6378(5)	3268(3)	1	45(2)
C(3)	3543(5)	5006(4)	4333(2)	1	34(2)
C(20)	4313(6)	-2504(5)	6763(3)	1	52(2)
C(21)	5169(6)	-2059(5)	6763(3)	1	49(2)
C(7)	2549(5)	6522(5)	3281(3)	1	44(2)
C(8)	2639(5)	7481(5)	3213(3)	1	48(2)
C(10)	4220(5)	7336(5)	3202(3)	1	52(2)
C(9)	3440(6)	7691(6)	2978(3)	1	55(2)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S8. Anisotropic displacement parameters (Å^2 × 10^3) for $(C_{11}H_{24}N_2)_2[In_{0.9}Sb_{0.1}Br_6][InBr_4]$ at 150 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
In(1)	28(1)	31(1)	33(1)	-1(1)	-1(1)	2(1)
Sb(1)	28(1)	31(1)	33(1)	-1(1)	-1(1)	2(1)
In(2)	44(1)	39(1)	37(1)	-2(1)	6(1)	2(1)
Br(4)	32(1)	35(1)	35(1)	-1(1)	0(1)	7(1)
Br(2)	34(1)	32(1)	37(1)	-1(1)	-2(1)	-2(1)
Br(6)	33(1)	37(1)	36(1)	2(1)	-1(1)	-4(1)
Br(3)	38(1)	35(1)	33(1)	0(1)	0(1)	-1(1)
Br(5)	41(1)	37(1)	37(1)	5(1)	-5(1)	-2(1)
Br(1)	35(1)	50(1)	42(1)	-1(1)	-2(1)	8(1)
Br(10)	45(1)	41(1)	48(1)	-1(1)	10(1)	6(1)
Br(9)	50(1)	42(1)	45(1)	1(1)	-4(1)	8(1)
Br(7)	103(1)	69(1)	38(1)	28(1)	16(1)	18(1)
Br(8)	45(1)	71(1)	130(2)	-15(1)	23(1)	-49(1)
N(1)	27(3)	31(3)	39(4)	-3(3)	-5(3)	4(3)
N(4)	32(3)	33(3)	37(4)	2(3)	3(3)	-2(3)
N(3)	28(3)	38(3)	40(4)	0(3)	-7(3)	6(3)

N(2)	36(4)	35(3)	25(3)	0(3)	4(3)	-1(3)
C(15)	34(4)	34(4)	38(5)	1(3)	-4(3)	-5(3)
C(13)	44(5)	27(4)	39(5)	-1(3)	3(4)	3(3)
C(16)	39(4)	36(4)	30(4)	1(3)	-7(3)	-2(3)
C(22)	44(5)	39(4)	40(5)	4(4)	-4(4)	2(4)
C(6)	37(4)	36(4)	31(4)	-1(3)	-3(3)	0(3)
C(18)	40(5)	38(4)	46(5)	-2(4)	3(4)	1(4)
C(14)	29(4)	33(4)	31(4)	1(3)	1(3)	0(3)
C(12)	44(5)	28(4)	41(5)	2(3)	6(4)	1(3)
C(17)	41(4)	29(4)	24(4)	5(3)	2(3)	1(3)
C(5)	39(5)	47(5)	33(5)	0(4)	-6(4)	12(4)
C(4)	40(4)	30(4)	33(4)	-6(3)	0(4)	-2(3)
C(19)	51(5)	33(4)	54(5)	-3(4)	-6(4)	-2(4)
C(1)	37(4)	42(4)	35(5)	3(4)	3(4)	-4(4)
C(2)	45(5)	28(4)	37(5)	-4(3)	-5(4)	-2(3)
C(11)	41(5)	49(5)	44(5)	12(4)	3(4)	8(4)
C(3)	35(4)	33(4)	34(4)	0(3)	3(3)	2(3)
C(20)	80(7)	38(4)	39(5)	4(5)	-1(5)	2(4)
C(21)	71(6)	37(4)	40(5)	19(4)	-18(4)	-5(4)
C(7)	49(5)	51(5)	33(5)	7(4)	-13(4)	1(4)
C(8)	48(5)	54(5)	42(5)	20(4)	1(4)	11(4)
C(10)	50(6)	50(5)	57(6)	7(4)	11(5)	24(4)
C(9)	58(6)	58(6)	49(6)	13(5)	18(5)	20(4)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S9. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $(C_{11}H_{24}N_2)_2[In_{0.8}Sb_{0.2}Br_6][InBr_4]$ at 150 K with estimated standard deviations in parentheses.

Label	*x*	*y*	*z*	Occupancy	U_{eq}*
In(1)	6331(1)	2179(1)	5213(1)	0.8	33(1)
Sb(1)	6331(1)	2179(1)	5213(1)	0.2	33(1)

In(2)	6365(1)	5113(1)	2989(1)	1	43(1)
Br(1)	6334(1)	3521(1)	4672(1)	1	37(1)
Br(5)	7454(1)	1316(1)	4732(1)	1	37(1)
Br(3)	5058(1)	1504(1)	4775(1)	1	39(1)
Br(6)	7743(1)	2934(1)	5555(1)	1	40(1)
Br(2)	5078(1)	3151(1)	5615(1)	1	44(1)
Br(4)	6336(1)	976(1)	5809(1)	1	47(1)
Br(8)	5048(1)	4462(1)	2694(1)	1	47(1)
Br(7)	6524(1)	6657(1)	2838(1)	1	49(1)
Br(9)	6316(1)	4950(1)	3778(1)	1	76(1)
Br(10)	7648(1)	4307(1)	2753(1)	1	87(1)
N(2)	8841(4)	4387(4)	3814(2)	1	33(2)
N(1)	8431(4)	3274(4)	4510(2)	1	40(2)
N(3)	4192(4)	3667(4)	4577(2)	1	36(2)
N(4)	3796(4)	4825(4)	3892(2)	1	38(2)
C(5)	9450(5)	4782(5)	3502(3)	1	40(2)
C(3)	8852(5)	3438(4)	3772(3)	1	38(2)
C(2)	9031(5)	4629(5)	4261(2)	1	34(2)
C(6)	9490(5)	5745(5)	3539(2)	1	36(2)
C(17)	3333(5)	6176(5)	3515(3)	1	39(2)
C(4)	8244(5)	3017(5)	4070(3)	1	43(2)
C(1)	8415(5)	4220(5)	4563(3)	1	38(2)
C(12)	4159(5)	4608(4)	4642(2)	1	36(2)
C(11)	10070(6)	6095(5)	3190(3)	1	47(2)
C(7)	8625(5)	6176(5)	3514(3)	1	43(2)
C(16)	3204(5)	5217(5)	3565(3)	1	44(2)
C(14)	3831(5)	3870(5)	3829(3)	1	41(2)
C(22)	4140(5)	6392(5)	3270(3)	1	45(2)
C(20)	3444(6)	7705(6)	2974(3)	1	55(2)
C(19)	2646(5)	7490(5)	3206(3)	1	46(2)

C(15)	4424(5)	3447(5)	4137(2)	1	42(2)
C(13)	3540(5)	5007(5)	4332(3)	1	38(2)
C(18)	2551(5)	6538(5)	3284(3)	1	47(2)
C(8)	8710(6)	7138(5)	3558(3)	1	50(2)
C(9)	9331(6)	7507(5)	3233(3)	1	58(2)
C(10)	10184(6)	7050(5)	3240(3)	1	55(2)
C(21)	4225(5)	7352(6)	3205(3)	1	55(2)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S10. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $(C_{11}H_{24}N_2)_2[In_{0.8}Sb_{0.2}Br_6][InBr_4]$ at 150 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
In(1)	31(1)	34(1)	36(1)	1(1)	0(1)	2(1)
Sb(1)	31(1)	34(1)	36(1)	1(1)	0(1)	2(1)
In(2)	46(1)	42(1)	42(1)	3(1)	-6(1)	2(1)
Br(1)	34(1)	38(1)	39(1)	0(1)	0(1)	6(1)
Br(5)	37(1)	35(1)	41(1)	1(1)	3(1)	-2(1)
Br(3)	36(1)	40(1)	39(1)	-2(1)	0(1)	-3(1)
Br(6)	45(1)	39(1)	38(1)	0(1)	1(1)	-1(1)
Br(2)	49(1)	43(1)	39(1)	-8(1)	6(1)	-2(1)
Br(4)	36(1)	57(1)	48(1)	0(1)	2(1)	8(1)
Br(8)	47(1)	44(1)	51(1)	1(1)	-8(1)	6(1)
Br(7)	52(1)	45(1)	50(1)	0(1)	4(1)	8(1)
Br(9)	115(1)	73(1)	42(1)	-32(1)	-20(1)	19(1)
Br(10)	48(1)	76(1)	137(2)	17(1)	-26(1)	-52(1)
N(2)	36(3)	31(3)	32(3)	1(3)	2(3)	0(3)
N(1)	34(3)	39(3)	46(4)	0(3)	4(3)	2(3)
N(3)	33(3)	30(3)	44(4)	-1(2)	-3(3)	6(3)
N(4)	42(3)	40(3)	33(4)	-1(3)	0(3)	1(3)
C(5)	33(4)	47(4)	40(5)	-2(3)	7(3)	2(4)

C(3)	46(4)	32(4)	38(5)	1(3)	-2(3)	4(3)
C(2)	40(4)	36(4)	26(4)	-2(3)	-2(3)	-4(3)
C(6)	44(4)	35(4)	30(4)	-5(3)	-3(3)	-5(3)
C(17)	36(4)	44(4)	37(5)	4(3)	-7(3)	1(3)
C(4)	37(4)	38(4)	54(5)	0(3)	-2(4)	0(4)
C(1)	37(4)	35(4)	42(5)	1(3)	6(3)	3(3)
C(12)	37(4)	32(4)	39(4)	-4(3)	-6(3)	0(3)
C(11)	57(5)	39(4)	46(5)	-9(4)	12(4)	-5(4)
C(7)	48(5)	35(4)	46(5)	-9(3)	5(4)	-6(4)
C(16)	42(4)	51(5)	38(5)	1(4)	-13(4)	7(4)
C(14)	50(5)	40(4)	33(4)	-5(3)	-1(4)	-2(3)
C(22)	46(5)	45(5)	44(5)	4(4)	5(4)	6(4)
C(20)	54(5)	60(6)	50(6)	11(4)	8(4)	15(4)
C(19)	46(5)	54(5)	38(5)	13(4)	9(4)	4(4)
C(15)	44(4)	45(4)	37(5)	5(4)	6(4)	-1(4)
C(13)	40(4)	33(4)	42(5)	-2(3)	-5(3)	-2(3)
C(18)	49(5)	55(5)	37(5)	3(4)	-6(4)	6(4)
C(8)	63(6)	33(4)	55(6)	7(4)	1(4)	1(4)
C(9)	77(6)	35(4)	63(6)	-6(4)	6(5)	6(4)
C(10)	73(6)	48(5)	43(5)	-18(4)	21(5)	-7(4)
C(21)	48(5)	55(5)	63(6)	5(4)	14(5)	18(5)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S11. Distortion degree of the $[In(Sb)Br_6]^{3-}$ octahedron and $[In(Sb)Br_4]^{-}$ tetrahedron for $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$:$xSb^{3+}$ (x = 0, 0.05 and 0.10) at 150 K.

x	0	0.05	0.10
λ_{oct}	1.69×10^{-4}	2.29×10^{-4}	3.09×10^{-4}
δ_{oct}^2	18.07	21.36	23.98
λ_{tet}	2.08×10^{-5}	1.95×10^{-5}	2.03×10^{-5}
δ_{tet}^2	10.25	9.96	9.57

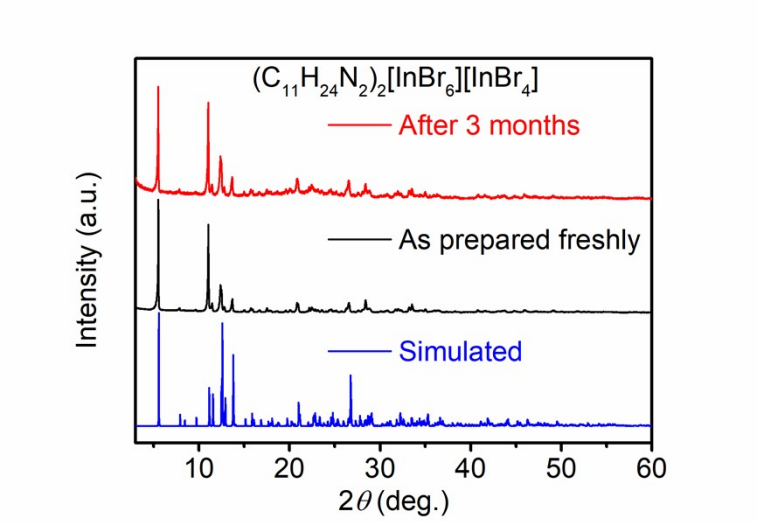

Figure S1. PXRD patterns of $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$ for simulation based on the singe-crystal refinements (blue), experimental data of fresh synthesized samples (black), and those in air for 3 months (red).

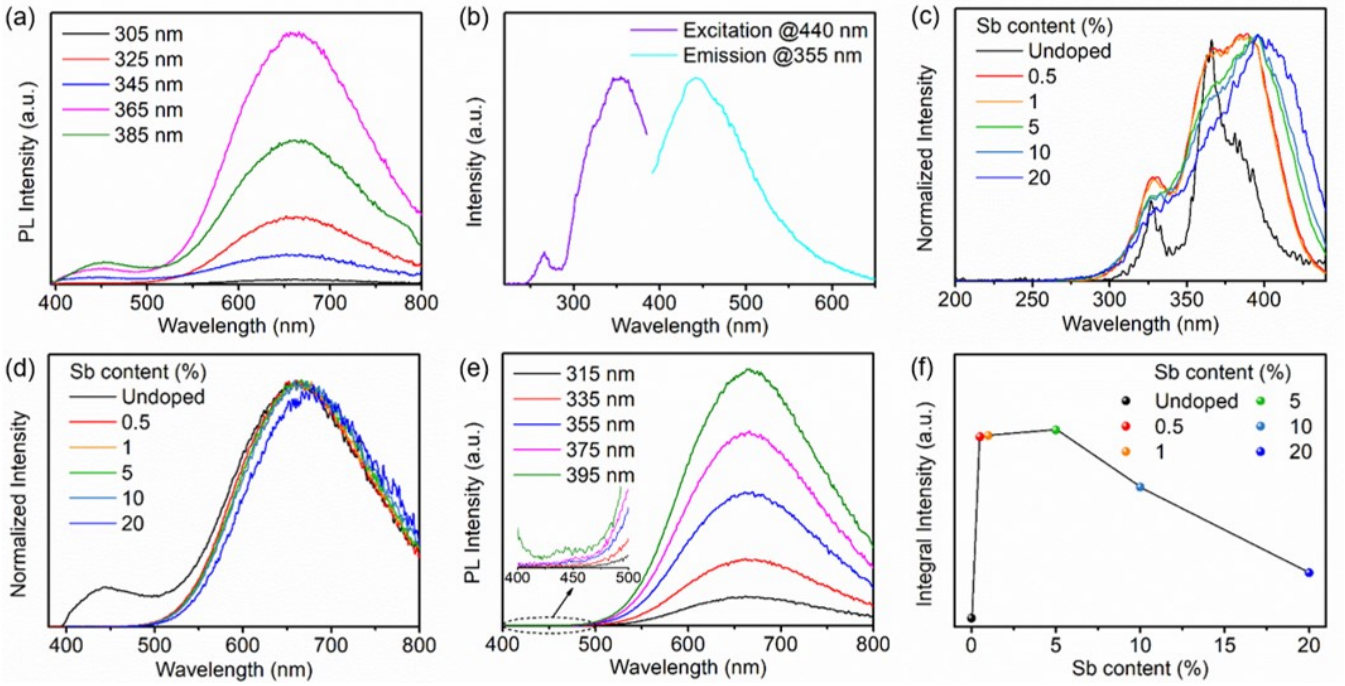

Figure S2. Emission spectra at different excitation wavelength of (a) $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$, and (e) $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$:5%$Sb^{3+}$. (b) Photoluminescent spectra of 1-(crylohexylmethyl)piperazine. Normalized (c) excitation and (d) emission spectra of $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$:*x*$Sb^{3+}$. (f) Integral PL intensity of $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$:*x*$Sb^{3+}$.

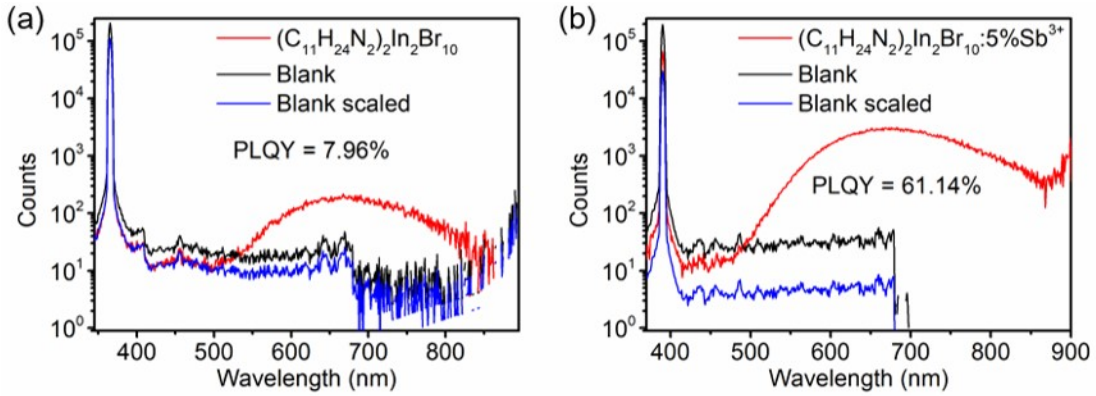

Figure S3. PLQY of (a) $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$, and (b) $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$:5%$Sb^{3+}$.

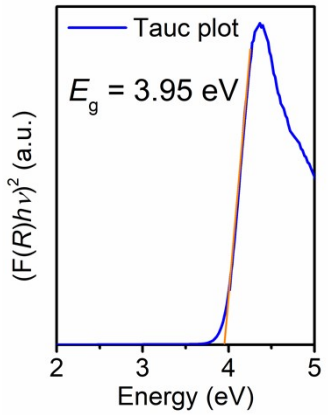

Figure S4. Band gap value of $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$ obtained from Tauc plot.[1]

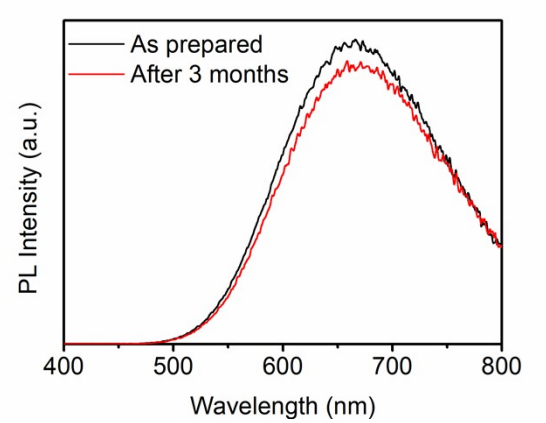

Figure S5. Comparison of the PL spectra of the as-prepared $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$:5%$Sb^{3+}$and the one exposed in the air for 3 months.

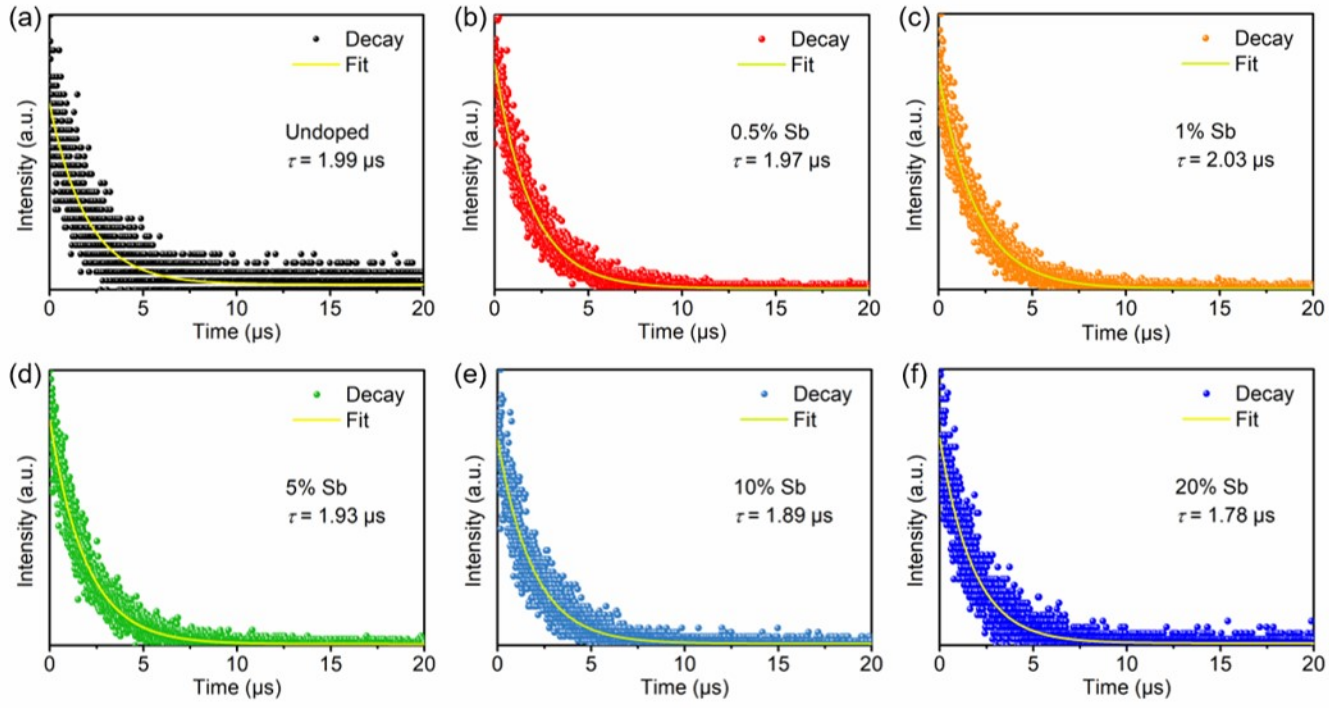

Figure S6. Time-resolved decay curves of $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$:$x$$Sb^{3+}$ by single exponential fit. (a)-(f) correspond x = 0, 0.005, 0.01, 0.05, 0.10, 0.20 in turn.

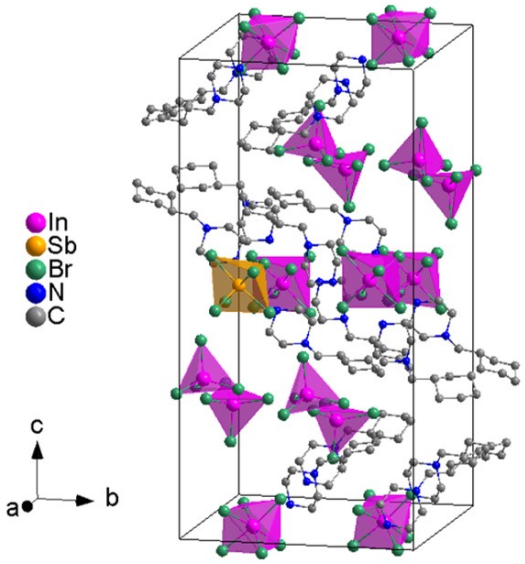

Figure S7. The structure model used for calculating the Sb-doped $(C_{11}H_{24}N_2)_2[InBr_6][InBr_4]$ (H atoms are omitted for charity). One of the eight In atoms in $[InBr_6]^{3-}$ octahedra was replaced by Sb atom, resulting in the formula $(C_{11}H_{24}N_2)_2[In_{0.875}Sb_{0.125}Br_6][InBr_4]$.

Reference

[1] J. Tauc, *Mater. Res. Bull.*, 1968, **3**, 37-46.