Supporting Information

Broadband Light Emitting Zero-Dimensional Antimony and Bismuth-Based Hybrid Halides with Diverse Structures

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Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **2** at 293(2) K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}^*
Bi(1)	6594(1)	-132(1)	3682(1)	1	11(1)
Bi(2)	7108(1)	5169(1)	6219(1)	1	12(1)
Br(5)	5576(1)	-2102(1)	3613(1)	1	17(1)
Br(8)	6163(1)	7117(1)	6211(1)	1	17(1)
Br(10)	8276(1)	3088(1)	6186(1)	1	18(1)
Br(1)	8253(1)	-385(1)	2951(1)	1	16(1)
Br(2)	7747(1)	1835(1)	3760(1)	1	19(1)
Br(6)	4690(1)	541(1)	3000(1)	1	18(1)
Br(7)	5806(1)	4645(1)	6986(1)	1	18(1)
Br(4)	4960(1)	255(1)	4355(1)	1	20(1)
Br(9)	4853(1)	4748(1)	5621(1)	1	19(1)
Br(12)	9255(1)	5775(1)	6807(1)	1	21(1)
Br(3)	8766(1)	-890(1)	4263(1)	1	23(1)
Br(11)	8506(1)	5537(1)	5462(1)	1	26(1)
N(5)	4393(5)	2830(4)	4924(2)	1	16(2)
N(1)	1507(5)	4526(4)	6352(2)	1	19(2)
N(4)	9048(6)	-559(5)	6385(2)	1	25(2)
N(3)	7246(5)	1503(5)	6929(2)	1	21(2)
N(2)	2070(5)	3144(4)	7464(2)	1	19(2)
N(6)	7997(5)	2409(4)	5117(2)	1	19(2)
C(9)	8784(7)	-1038(6)	5928(2)	1	25(2)
C(2)	1571(6)	3776(6)	5985(2)	1	21(2)
C(10)	8922(7)	-1334(6)	6738(2)	1	27(2)
O(00)	5581(7)	3132(5)	2889(2)	1	56(2)
C(7)	8381(6)	860(5)	6869(2)	1	18(2)
C(3)	2194(6)	4212(5)	6791(2)	1	17(2)
C(12)	5624(6)	2397(5)	5129(2)	1	16(2)
C(5)	3407(6)	2742(5)	7511(2)	1	18(2)
C(1)	2011(7)	5508(6)	6216(2)	1	27(2)
C(8)	8196(7)	318(6)	6419(2)	1	23(2)
C(15)	9111(6)	2899(6)	4938(2)	1	23(2)
C(11)	3263(6)	2300(6)	5086(2)	1	25(2)
C(6)	7414(7)	2148(6)	7339(2)	1	28(2)
C(4)	1506(6)	3325(6)	6994(2)	1	21(2)
C(13)	6757(6)	2847(5)	4914(2)	1	19(2)

C(14)	8063(7)	1283(6)	5054(2)	1	25(2)

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

Table S2. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2** at 293(2) K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Bi(1)	11(1)	10(1)	11(1)	0(1)	1(1)	0(1)
Bi(2)	13(1)	11(1)	12(1)	1(1)	3(1)	0(1)
Br(5)	18(1)	12(1)	20(1)	-1(1)	-1(1)	0(1)
Br(8)	22(1)	12(1)	16(1)	2(1)	3(1)	0(1)
Br(10)	26(1)	12(1)	15(1)	3(1)	3(1)	0(1)
Br(1)	16(1)	16(1)	16(1)	1(1)	4(1)	-2(1)
Br(2)	27(1)	12(1)	18(1)	-4(1)	2(1)	-2(1)
Br(6)	16(1)	21(1)	17(1)	-2(1)	-2(1)	5(1)
Br(7)	22(1)	17(1)	16(1)	-2(1)	7(1)	1(1)
Br(4)	24(1)	22(1)	15(1)	1(1)	7(1)	-2(1)
Br(9)	19(1)	21(1)	18(1)	-2(1)	-1(1)	-4(1)
Br(12)	16(1)	22(1)	25(1)	3(1)	-2(1)	-7(1)
Br(3)	19(1)	21(1)	29(1)	-2(1)	-8(1)	7(1)
Br(11)	31(1)	24(1)	27(1)	1(1)	16(1)	6(1)
N(5)	20(3)	16(3)	12(3)	1(2)	0(2)	0(2)
N(1)	19(3)	18(3)	21(3)	-2(3)	2(2)	-2(2)
N(4)	24(3)	17(3)	32(3)	-3(3)	-2(3)	-2(3)
N(3)	11(3)	24(4)	28(3)	-1(3)	2(2)	5(3)
N(2)	25(3)	11(3)	20(3)	2(3)	4(2)	1(2)
N(6)	22(3)	16(3)	18(3)	-1(3)	0(2)	-3(2)
C(9)	31(4)	20(4)	24(4)	3(3)	2(3)	-4(3)
C(2)	19(4)	21(4)	23(4)	-3(3)	3(3)	-5(3)
C(10)	36(4)	17(4)	24(4)	0(3)	-11(3)	4(3)
O(00)	83(5)	32(4)	61(4)	30(4)	54(4)	18(3)
C(7)	16(3)	9(4)	27(4)	1(3)	-6(3)	4(3)
C(3)	20(4)	12(4)	20(3)	-5(3)	0(3)	0(3)
C(12)	19(3)	14(4)	14(3)	6(3)	-3(3)	2(3)
C(5)	17(3)	18(4)	20(3)	4(3)	2(3)	2(3)
C(1)	30(4)	24(5)	30(4)	-3(3)	9(3)	5(3)
C(8)	21(4)	25(5)	23(4)	13(3)	-3(3)	9(3)
C(15)	20(4)	24(4)	26(4)	-2(3)	7(3)	-6(3)
C(11)	17(4)	30(5)	29(4)	-3(3)	3(3)	1(3)
C(6)	38(5)	23(5)	24(4)	7(4)	6(3)	-1(3)
C(4)	19(4)	21(4)	23(4)	-1(3)	-1(3)	3(3)
C(13)	22(4)	18(4)	16(3)	3(3)	0(3)	-1(3)

C(14)	26(4)	21(4)	28(4)	0(3)	-2(3)	3(3)

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

Table S3. Bond lengths [Å] for **2** at 293(2) K with estimated standard deviations in parentheses.

Label	Distances	Label	Distances
Bi(1)-Br(5)	2.8228(7)	N(1)-C(3)	1.489(8)
Bi(1)-Br(1)	2.9353(6)	N(1)-C(1)	1.478(9)
Bi(1)-Br(2)	2.8755(7)	N(4)-C(9)	1.505(9)
Bi(1)-Br(6)	2.8452(7)	N(4)-C(10)	1.490(9)
Bi(1)-Br(4)	2.8082(7)	N(4)-C(8)	1.474(9)
Bi(1)-Br(3)	2.8947(7)	N(3)-C(7)	1.484(8)
Bi(2)-Br(8)	2.7672(7)	N(3)-C(6)	1.489(9)
Bi(2)-Br(10)	3.0262(7)	N(2)-C(5)	1.487(8)
Bi(2)-Br(7)	2.8610(6)	N(2)-C(4)	1.487(8)
Bi(2)-Br(9)	2.8627(7)	N(6)-C(15)	1.477(8)
Bi(2)-Br(12)	2.8225(7)	N(6)-C(13)	1.491(8)
Bi(2)-Br(11)	2.8498(7)	N(6)-C(14)	1.510(9)
N(5)-C(12)	1.482(8)	C(7)-C(8)	1.520(9)
N(5)-C(11)	1.493(8)	C(3)-C(4)	1.536(9)
N(1)-C(2)	1.486(8)	C(12)-C(13)	1.522(9)

Symmetry transformations used to generate equivalent atoms:

Table S4. Bond angles [°] for **2** at 293(2) K with estimated standard deviations in parentheses.

Label	Angles	Label	Angles
Br(5)-Bi(1)-Br(1)	94.89(2)	Br(12)-Bi(2)-Br(7)	88.95(2)
Br(5)-Bi(1)-Br(2)	177.39(2)	Br(12)-Bi(2)-Br(9)	174.61(2)
Br(5)-Bi(1)-Br(6)	90.48(2)	Br(12)-Bi(2)-Br(11)	90.41(2)
Br(5)-Bi(1)-Br(3)	89.30(2)	Br(11)-Bi(2)-Br(10)	83.77(2)
Br(2)-Bi(1)-Br(1)	83.786(19)	Br(11)-Bi(2)-Br(7)	175.36(2)
Br(2)-Bi(1)-Br(3)	88.35(2)	Br(11)-Bi(2)-Br(9)	89.62(2)
Br(6)-Bi(1)-Br(1)	85.697(19)	C(12)-N(5)-C(11)	111.3(5)
Br(6)-Bi(1)-Br(2)	91.66(2)	C(2)-N(1)-C(3)	114.1(5)
Br(6)-Bi(1)-Br(3)	171.17(2)	C(1)-N(1)-C(2)	110.2(5)
Br(4)-Bi(1)-Br(5)	88.32(2)	C(1)-N(1)-C(3)	109.6(5)
Br(4)-Bi(1)-Br(1)	175.67(2)	C(10)-N(4)-C(9)	109.2(6)
Br(4)-Bi(1)-Br(2)	93.11(2)	C(8)-N(4)-C(9)	109.8(5)
Br(4)-Bi(1)-Br(6)	91.39(2)	C(8)-N(4)-C(10)	113.7(6)
Br(4)-Bi(1)-Br(3)	97.43(2)	C(7)-N(3)-C(6)	113.6(5)
Br(3)-Bi(1)-Br(1)	85.53(2)	C(4)-N(2)-C(5)	115.2(5)
Br(8)-Bi(2)-Br(10)	176.10(2)	C(15)-N(6)-C(13)	111.3(5)
Br(8)-Bi(2)-Br(7)	92.11(2)	C(15)-N(6)-C(14)	110.2(5)
Br(8)-Bi(2)-Br(9)	84.70(2)	C(13)-N(6)-C(14)	112.6(5)
Br(8)-Bi(2)-Br(12)	89.92(2)	N(3)-C(7)-C(8)	110.3(5)
Br(8)-Bi(2)-Br(11)	92.48(2)	N(1)-C(3)-C(4)	111.0(5)
Br(7)-Bi(2)-Br(10)	91.63(2)	N(5)-C(12)-C(13)	110.5(5)
Br(7)-Bi(2)-Br(9)	91.45(2)	N(4)-C(8)-C(7)	114.2(5)
Br(9)-Bi(2)-Br(10)	96.32(2)	N(2)-C(4)-C(3)	109.9(5)
Br(12)-Bi(2)-Br(10)	89.04(2)	N(6)-C(13)-C(12)	110.8(5)

Symmetry transformations used to generate equivalent atoms:

Table S5. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **3** at 293(2) K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}*
Sb(1)	6359(1)	5164(1)	3884(1)	1	20(1)
Sb(2)	8349(1)	7500	8657(1)	1	22(1)
Sb(3)	9991(1)	5862(1)	2362(1)	1	21(1)
Sb(4)	6631(1)	7500	7908(1)	1	27(1)
Cl(1)	6809(1)	4532(1)	3020(2)	1	37(1)
Cl(2)	7016(1)	5232(1)	5656(2)	1	34(1)
Cl(3)	9335(1)	5804(1)	4197(2)	1	36(1)
Cl(4)	8501(1)	7500	11458(2)	1	38(1)
Cl(5)	8355(1)	7500	6158(2)	1	25(1)
Cl(6)	6904(1)	7500	5449(2)	1	41(1)
Cl(7)	5816(1)	5951(1)	4806(2)	1	37(1)
Cl(8)	10553(1)	5139(1)	3464(2)	1	30(1)
Cl(9)	9479(1)	6488(1)	1576(2)	1	49(1)
Cl(10)	10608(1)	6308(1)	3753(2)	1	34(1)
Cl(11)	6927(1)	5618(1)	2446(2)	1	35(1)
Cl(12)	7475(1)	6853(1)	8447(2)	1	37(1)
Cl(13)	9348(1)	5321(1)	684(2)	1	43(1)
Cl(14)	6286(1)	7500	10477(2)	1	45(1)
Cl(15)	5968(1)	6930(1)	7469(2)	1	56(1)
Cl(16)	9035(1)	6941(1)	8594(2)	1	57(1)
N(1)	8010(2)	6506(2)	1570(3)	1	27(1)
N(3)	9943(2)	4340(2)	2166(3)	1	25(1)
N(4)	8659(2)	4511(2)	4230(3)	1	26(1)
N(5)	7730(2)	6619(2)	5214(3)	1	30(1)
C(7)	8044(2)	6382(2)	2983(4)	1	25(1)
C(8)	9522(2)	4243(2)	3178(4)	1	28(1)
C(9)	8333(2)	4122(2)	3930(5)	1	36(2)
C(10)	8289(2)	4892(2)	4331(5)	1	36(2)
C(11)	10364(2)	3998(2)	2062(5)	1	36(2)
C(13)	7888(2)	6756(2)	3857(4)	1	28(1)
C(15)	8163(3)	6358(2)	5867(5)	1	57(2)
C(16)	9100(2)	4597(2)	3233(4)	1	28(1)
C(17)	8148(2)	6145(2)	674(5)	1	31(1)
C(18)	7175(2)	6408(2)	5236(6)	1	54(2)
O(1)	6898(2)	6677(2)	1727(4)	1	50(1)

N(2)	9990(3)	7500	4821(7)	1	75(2)
N(6)	9936(3)	7500	1115(7)	1	75(2)
C(3)	10152(4)	7500	2430(9)	1	75(2)
C(1B)	10821(5)	6935(5)	885(12)	0.50	75(2)
C(19)	10263(5)	7298(5)	35(11)	0.50	75(2)
C(2)	9794(5)	7125(5)	5560(12)	0.50	75(2)
C(4)	9824(4)	7500	3452(9)	1	75(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 **3** at 293(2) K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sb(1)	21(1)	23(1)	17(1)	-2(1)	1(1)	1(1)
Sb(2)	25(1)	22(1)	19(1)	0	-2(1)	0
Sb(3)	21(1)	23(1)	19(1)	0(1)	-3(1)	1(1)
Sb(4)	22(1)	26(1)	32(1)	0	1(1)	0
Cl(1)	47(1)	28(1)	36(1)	6(1)	6(1)	-5(1)
Cl(2)	27(1)	52(1)	24(1)	6(1)	-5(1)	-5(1)
Cl(3)	29(1)	48(1)	32(1)	0(1)	7(1)	2(1)
Cl(4)	57(1)	30(1)	26(1)	0	5(1)	0
Cl(5)	31(1)	25(1)	20(1)	0	-3(1)	0
Cl(6)	41(1)	40(1)	41(1)	0	0(1)	0
Cl(7)	41(1)	38(1)	33(1)	-6(1)	7(1)	-6(1)
Cl(8)	32(1)	32(1)	25(1)	-5(1)	-3(1)	0(1)
Cl(9)	42(1)	38(1)	66(1)	0(1)	-21(1)	19(1)
Cl(10)	31(1)	39(1)	33(1)	-9(1)	-6(1)	-3(1)
Cl(11)	42(1)	35(1)	29(1)	-14(1)	7(1)	0(1)
Cl(12)	41(1)	29(1)	39(1)	-1(1)	1(1)	1(1)
Cl(13)	51(1)	38(1)	40(1)	-8(1)	-4(1)	6(1)
Cl(14)	33(1)	46(1)	56(2)	0	2(1)	0
Cl(15)	55(1)	51(1)	62(1)	-27(1)	-9(1)	4(1)
Cl(16)	67(1)	69(1)	36(1)	46(1)	-7(1)	-2(1)
N(1)	32(2)	25(2)	23(2)	-1(2)	1(2)	-4(2)
N(3)	25(2)	26(2)	23(2)	-4(2)	3(2)	2(2)
N(4)	21(2)	37(2)	18(2)	0(2)	-1(2)	0(2)
N(5)	45(2)	22(2)	22(2)	-5(2)	7(2)	-6(2)
C(7)	26(2)	27(2)	22(2)	1(2)	0(2)	0(2)
C(8)	26(2)	33(2)	24(2)	-3(2)	4(2)	3(2)
C(9)	30(2)	42(3)	34(3)	-10(2)	1(2)	-4(2)
C(10)	29(2)	44(3)	34(3)	8(2)	4(2)	-4(2)
C(11)	33(2)	42(3)	33(3)	10(2)	3(2)	-1(2)
C(13)	38(2)	25(2)	23(2)	-2(2)	1(2)	-1(2)
C(15)	92(4)	50(3)	28(3)	25(3)	1(3)	2(3)
C(16)	26(2)	34(2)	24(2)	2(2)	4(2)	3(2)
C(17)	32(2)	33(2)	28(2)	3(2)	-1(2)	-5(2)
C(18)	63(3)	49(3)	49(3)	-29(3)	26(3)	-22(3)
O(1)	35(2)	52(2)	63(3)	4(2)	-10(2)	9(2)

N(2)	54(2)	132(4)	40(2)	0	3(2)	0
N(6)	54(2)	132(4)	40(2)	0	3(2)	0
C(3)	54(2)	132(4)	40(2)	0	3(2)	0
C(1B)	54(2)	132(4)	40(2)	0	3(2)	0
C(19)	54(2)	132(4)	40(2)	0	3(2)	0
C(2)	54(2)	132(4)	40(2)	0	3(2)	0
C(4)	54(2)	132(4)	40(2)	0	3(2)	0

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

Table S7. Bond lengths [Å] for **3** at 293(2) K with estimated standard deviations in parentheses.

Label	Distances	Label	Distances
Sb(1)-Cl(1)	2.4302(11)	N(3)-C(11)	1.488(5)
Sb(1)-Cl(2)	2.4101(11)	N(4)-C(9)	1.489(6)
Sb(1)-Cl(11)	2.4624(11)	N(4)-C(10)	1.502(5)
Sb(2)-Cl(4)	2.8618(17)	N(4)-C(16)	1.496(5)
Sb(2)-Cl(5)	2.5321(14)	N(5)-C(13)	1.492(5)
Sb(2)-Cl(16)#1	2.4225(12)	N(5)-C(15)	1.488(6)
Sb(2)-Cl(16)	2.4225(12)	N(5)-C(18)	1.503(6)
Sb(3)-Cl(3)	2.4552(11)	C(7)-C(13)	1.521(6)
Sb(3)-Cl(8)	2.8775(11)	C(8)-C(16)	1.515(6)
Sb(3)-Cl(9)	2.4593(12)	N(2)-C(2)#1	1.475(15)
Sb(3)-Cl(10)	2.4883(11)	N(2)-C(2)	1.475(15)
Sb(3)-Cl(13)	2.8675(13)	N(2)-C(4)	1.444(11)
Sb(4)-Cl(6)	2.5773(19)	N(6)-C(3)	1.432(11)
Sb(4)-Cl(14)	2.735(2)	N(6)-C(19)	1.493(13)
Sb(4)-Cl(15)#1	2.4512(13)	N(6)-C(19)#1	1.493(13)
Sb(4)-Cl(15)	2.4512(13)	C(3)-C(4)	1.307(13)
N(1)-C(7)	1.486(5)	C(1B)-C(19)	1.970(19)
N(1)-C(17)	1.491(5)	C(19)-C(19)#1	1.27(3)
N(3)-C(8)	1.480(5)		

Symmetry transformations used to generate equivalent atoms:
(1) x,-y+3/2,z

Table S8. Bond angles [°] for **3** at 293(2) K with estimated standard deviations in parentheses.

Label	Angles	Label	Angles
Cl(1)-Sb(1)-Cl(11)	90.55(4)	Cl(15)-Sb(4)-Cl(15)#1	94.00(8)
Cl(2)-Sb(1)-Cl(1)	92.47(4)	C(7)-N(1)-C(17)	112.0(3)
Cl(2)-Sb(1)-Cl(11)	91.10(4)	C(8)-N(3)-C(11)	112.0(3)
Cl(5)-Sb(2)-Cl(4)	172.27(5)	C(9)-N(4)-C(10)	110.6(3)
Cl(16)#1-Sb(2)-Cl(4)	86.42(4)	C(9)-N(4)-C(16)	113.1(3)
Cl(16)-Sb(2)-Cl(4)	86.42(4)	C(16)-N(4)-C(10)	109.2(3)
Cl(16)#1-Sb(2)-Cl(5)	88.26(4)	C(13)-N(5)-C(18)	112.0(4)
Cl(16)-Sb(2)-Cl(5)	88.26(4)	C(15)-N(5)-C(13)	112.8(4)
Cl(16)-Sb(2)-Cl(16)#1	93.07(9)	C(15)-N(5)-C(18)	112.6(4)
Cl(3)-Sb(3)-Cl(8)	87.43(4)	N(1)-C(7)-C(13)	110.1(3)
Cl(3)-Sb(3)-Cl(9)	88.65(5)	N(3)-C(8)-C(16)	109.9(3)
Cl(3)-Sb(3)-Cl(10)	90.24(4)	N(5)-C(13)-C(7)	112.0(3)
Cl(3)-Sb(3)-Cl(13)	92.94(4)	N(4)-C(16)-C(8)	112.0(3)
Cl(9)-Sb(3)-Cl(8)	175.88(4)	C(2)-N(2)-C(2)#1	106.0(12)
Cl(9)-Sb(3)-Cl(10)	92.18(4)	C(4)-N(2)-C(2)#1	113.4(6)
Cl(9)-Sb(3)-Cl(13)	90.38(4)	C(4)-N(2)-C(2)	113.4(6)
Cl(10)-Sb(3)-Cl(8)	86.57(3)	C(3)-N(6)-C(19)#1	119.2(7)
Cl(10)-Sb(3)-Cl(13)	175.96(4)	C(3)-N(6)-C(19)	119.2(7)
Cl(13)-Sb(3)-Cl(8)	91.09(3)	C(19)-N(6)-C(19)#1	50.3(12)
Cl(6)-Sb(4)-Cl(14)	177.06(5)	C(4)-C(3)-N(6)	120.9(9)
Cl(15)#1-Sb(4)-Cl(6)	89.64(5)	N(6)-C(19)-C(1B)	106.9(8)
Cl(15)-Sb(4)-Cl(6)	89.64(5)	C(19)#1-C(19)-N(6)	64.9(6)
Cl(15)-Sb(4)-Cl(14)	88.35(5)	C(19)#1-C(19)-C(1B)	125.4(6)
Cl(15)#1-Sb(4)-Cl(14)	88.35(5)	C(3)-C(4)-N(2)	126.1(9)

Symmetry transformations used to generate equivalent atoms:
(1) x,-y+3/2,z

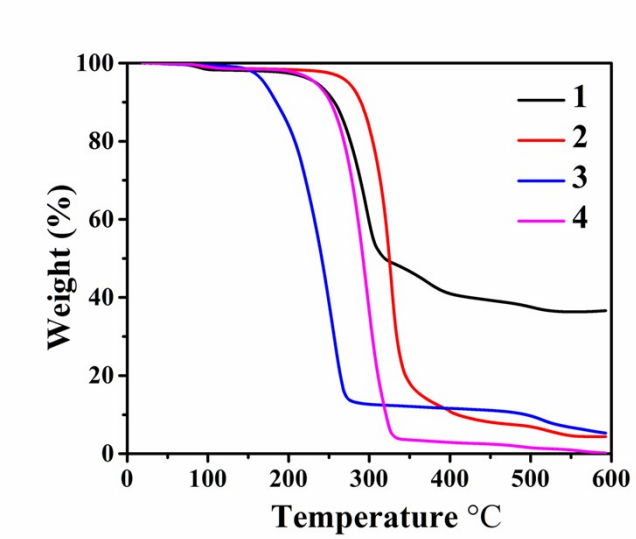

Figure S1. TGA curves of the obtained OIMHs **1-4**.

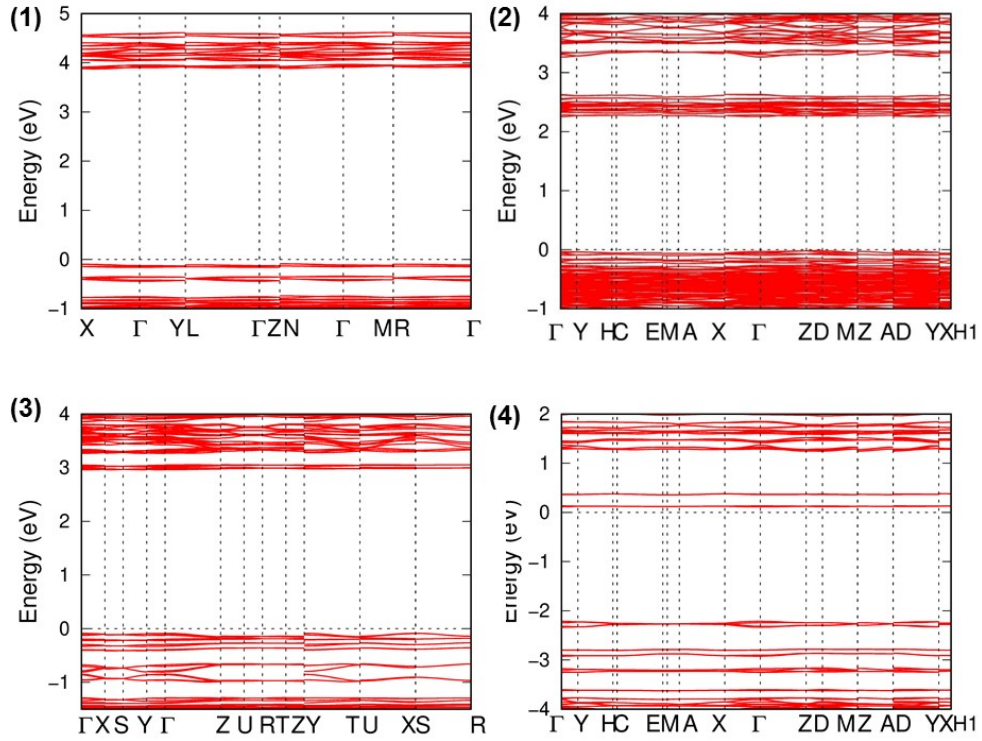

Figure S2. Band structures of compounds **1-4**.

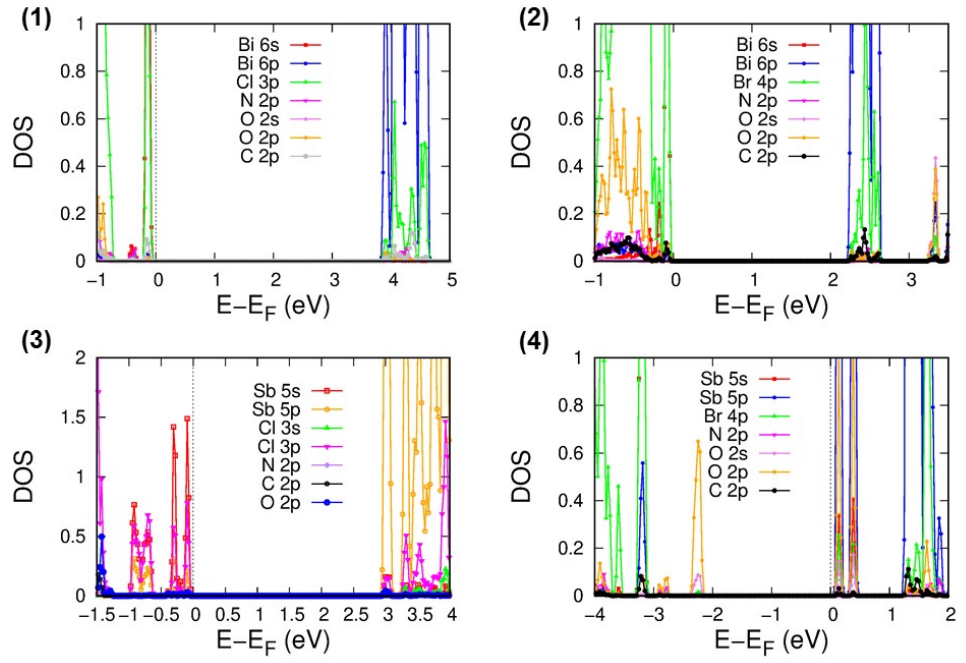

Figure S3. Densities of states and their orbital projections compounds **1-4**.

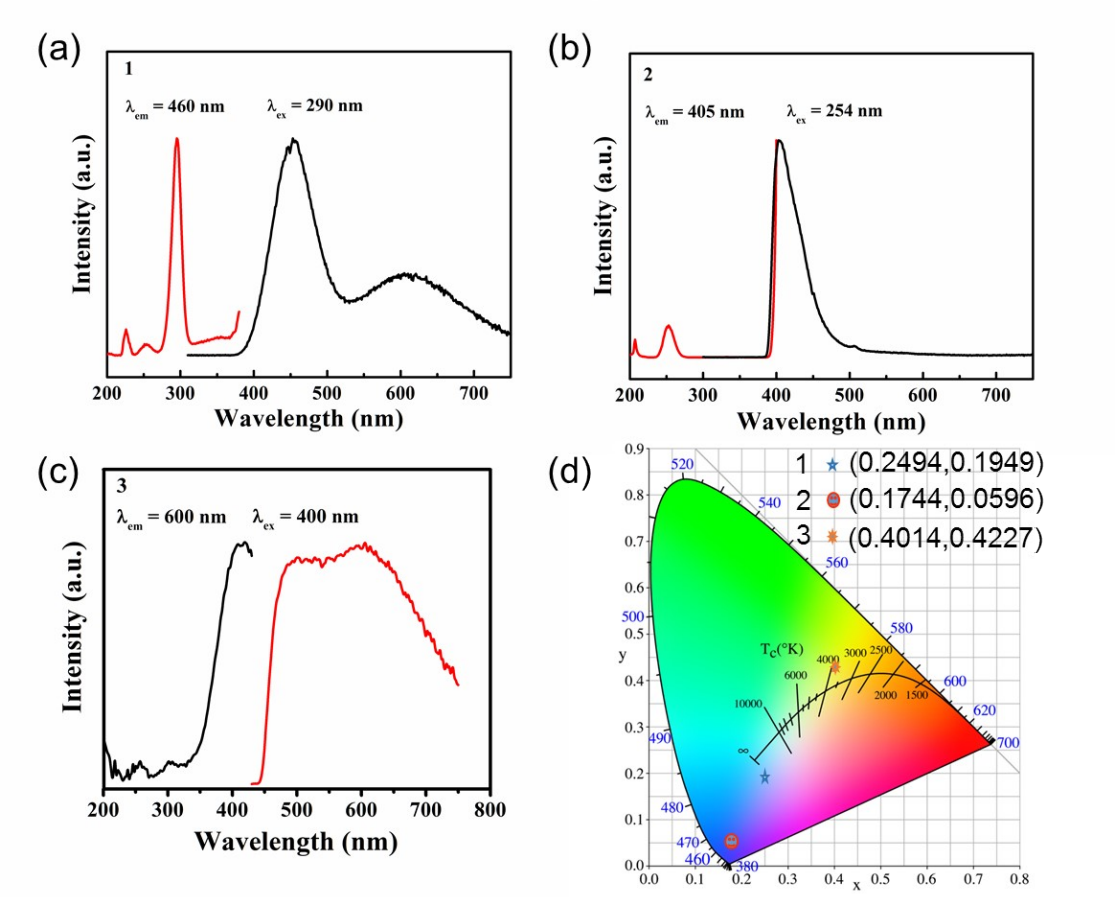

Figure S4. PLE and PL spectra of (a) **1**, (b) **2** and (c) **3** at RT. (d) CIE color coordinates of **1-3**.

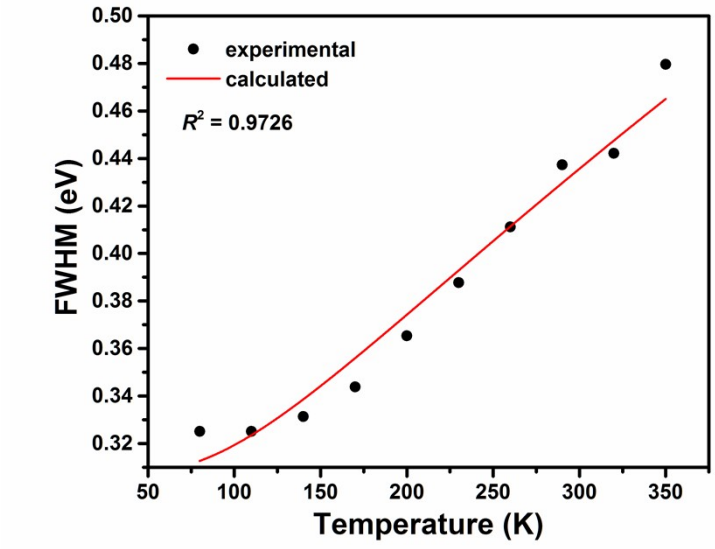

Figure S5. Fitting of the FWHM for compound **4** as a function of temperature.