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Electronic Supplementary Information (ESI)

for

Insight on noncovalent interactions and orbital constructs in low-dimensional antimony halide perovskites

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Electronic Supplementary Information Section

Figure S1. ORTEP drawing of compound **1**, $(C_5H_6N)[SbCl_4]$.

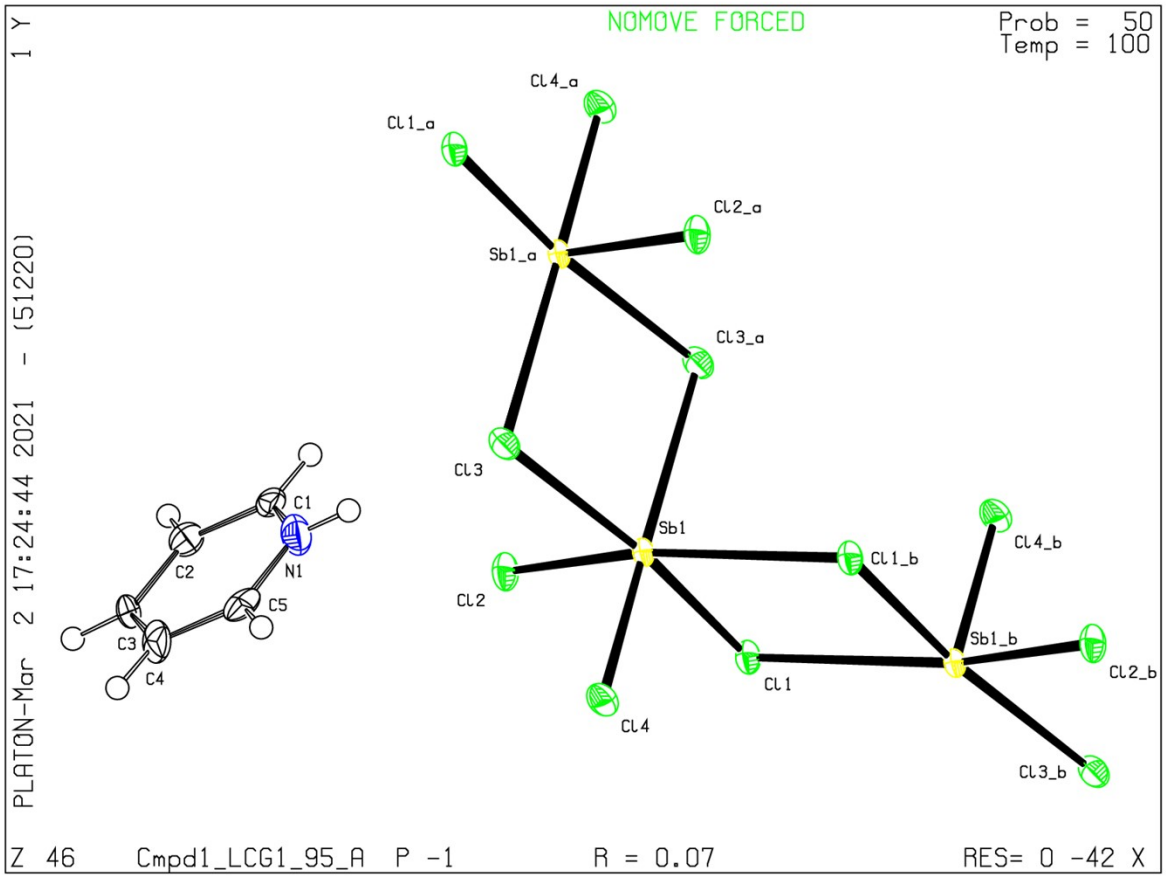

Table S1. Bond distances and angles for compound **1**, $(C_5H_6N)[SbCl_4]$.

Atom1	Atom2	Length (Å)	Atom1	Atom2	Atom3	Angle (°)
Sb1	Cl1	2.528(3)	N1	C5	C4	118(1)
Sb1	Cl2	2.393(4)	N1	C1	C2	120(1)
Sb1	Cl3	2.849(4)	Cl3	Sb1	Cl4	87.9(1)
Sb1	Cl4	2.420(4)	Cl2	Sb1	Cl3	84.69(9)
N1	C1	1.34(2)	Cl2	Sb1	Cl4	94.3(1)
N1	C5	1.35(2)	Cl1	Sb1	Cl2	88.6(1)
C4	C5	1.38(2)	Cl1	Sb1	Cl3	172.93(9)
C3	C4	1.39(2)	Cl1	Sb1	Cl4	90.5(1)
C2	C3	1.38(2)	C3	C4	C5	122(1)
C1	C2	1.38(2)	C2	C3	C4	118(1)
			C1	N1	C5	122(1)
			C1	C2	C3	120(1)

Figure S2. ORTEP drawing of compound **2**, $(C_5H_5NCl)[Sb_2Cl_9]$.

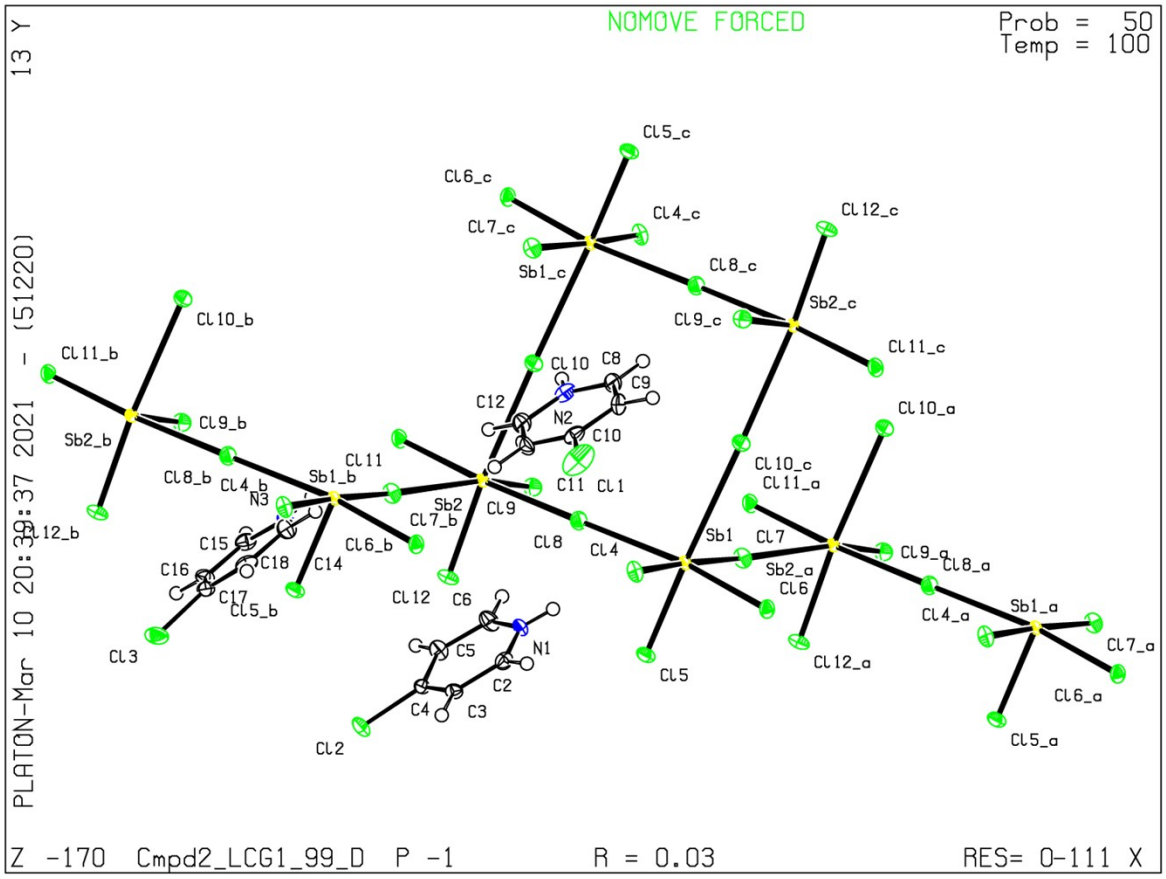

Table S2. Bond distances and angles for compound **2**, $(C_5H_5NCl)[Sb_2Cl_9]$.

Atom1	Atom2	Length (Å)	Atom1	Atom2	Atom3	Angle (°)
Sb2	Cl10	3.0044(7)	Sb1	Cl8	Sb2	178.22(3)
Sb2	Cl11	2.5067(8)	N3	C18	C17	119.3(2)
Sb2	Cl12	2.4136(7)	N3	C14	C15	120.2(3)
Sb2	Cl8	2.7725(8)	N2	C8	C9	119.9(3)
Sb2	Cl9	2.3887(8)	N2	C12	C11	120.4(3)
Sb1	Cl4	2.6412(8)	N1	C6	C5	119.8(3)
Sb1	Cl5	2.4092(7)	N1	C2	C3	119.6(2)
Sb1	Cl6	2.4312(8)	Cl9	Sb2	Cl10	84.94(2)
Sb1	Cl7	2.6098(8)	Cl9	Sb2	Cl11	88.42(3)
Sb1	Cl8	2.9879(8)	Cl9	Sb2	Cl12	89.76(3)
N3	C14	1.331(5)	Cl8	Sb2	Cl10	87.20(2)
N3	C18	1.341(3)	Cl8	Sb2	Cl11	175.69(2)
N2	C12	1.331(4)	Cl8	Sb2	Cl12	90.60(2)
N2	C8	1.337(4)	Cl8	Sb2	Cl9	89.02(2)
N1	C2	1.343(4)	Cl7	Sb1	Cl8	92.03(2)
N1	C6	1.336(5)	Cl6	Sb1	Cl7	88.45(2)
Cl3	C16	1.719(3)	Cl6	Sb1	Cl8	173.18(2)
Cl2	C4	1.716(3)	Cl5	Sb1	Cl6	90.68(3)
Cl1	C10	1.719(4)	Cl5	Sb1	Cl7	91.24(2)
C9	C10	1.374(4)	Cl5	Sb1	Cl8	82.51(2)
C8	C9	1.363(5)	Cl4	Sb1	Cl5	89.33(2)
C5	C6	1.373(4)	Cl4	Sb1	Cl6	86.44(2)
C4	C5	1.383(4)	Cl4	Sb1	Cl7	174.86(2)
C3	C4	1.383(4)	Cl4	Sb1	Cl8	93.11(2)
C2	C3	1.372(4)	Cl3	C16	C15	119.9(2)
C17	C18	1.364(4)	Cl3	C16	C17	119.3(2)
C16	C17	1.387(5)	Cl2	C4	C3	119.0(2)
C15	C16	1.387(5)	Cl2	C4	C5	120.3(2)
C14	C15	1.378(4)	Cl11	Sb2	Cl12	92.84(3)
C11	C12	1.363(5)	Cl10	Sb2	Cl11	89.13(2)
C10	C11	1.381(5)	Cl10	Sb2	Cl12	174.29(2)
			Cl1	C10	C11	118.8(2)
			Cl1	C10	C9	120.1(2)
			C9	C10	C11	121.1(3)
			C8	N2	C12	122.4(3)
			C8	C9	C10	118.4(3)
			C4	C5	C6	118.5(3)
			C3	C4	C5	120.7(3)
			C2	N1	C6	122.8(3)
			C2	C3	C4	118.5(2)
			C16	C17	C18	119.0(3)
			C15	C16	C17	120.8(3)
			C14	N3	C18	123.1(3)
			C14	C15	C16	117.6(3)
			C10	C11	C12	117.9(3)

Figure S3. ORTEP drawing of compound **3**, $(C_5H_5NBr)[Sb_2Cl_9]$.

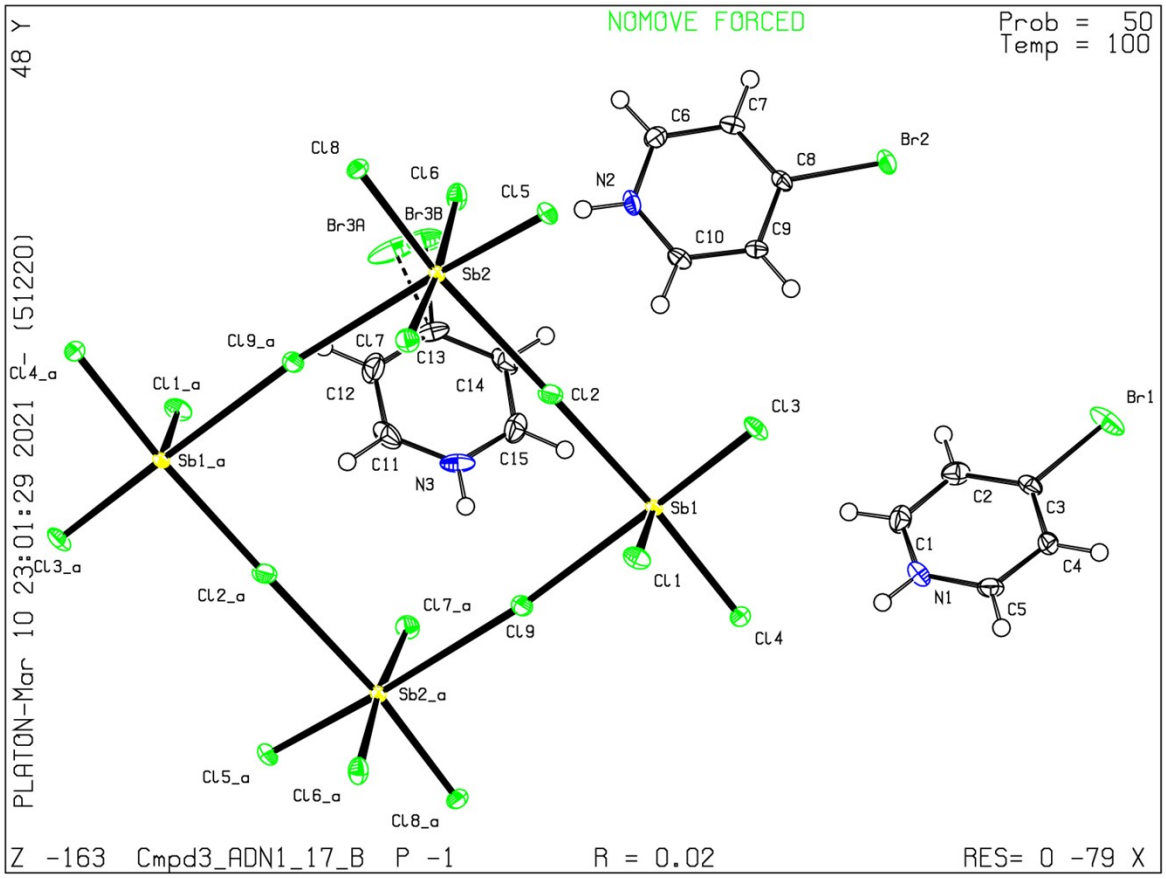

Table S3. Bond distances and angles for compound **3**, $(C_5H_5NBr)[Sb_2Cl_9]$.

Atom1	Atom2	Length (Å)	Atom1	Atom2	Atom3	Angle (°)
Sb2	Cl5	2.4082(6)	Sb1	Cl2	Sb2	178.03(3)
Sb2	Cl6	2.6400(8)	N3	C15	C14	120.1(3)
Sb2	Cl7	2.6135(7)	N3	C11	C12	119.7(3)
Sb2	Cl8	2.4259(7)	N2	C6	C7	119.7(2)
Sb1	Cl1	2.3839(7)	N2	C10	C9	120.1(2)
Sb1	Cl2	2.7745(8)	N1	C5	C4	119.6(2)
Sb1	Cl3	2.4170(6)	N1	C1	C2	120.1(2)
Sb1	Cl4	2.5052(7)	Cl7	Sb2	Cl8	88.47(2)
Sb1	Cl9	2.9896(7)	Cl6	Sb2	Cl7	174.54(2)
N3	C11	1.331(4)	Cl6	Sb2	Cl8	86.13(2)
N3	C15	1.330(4)	Cl5	Sb2	Cl6	89.57(2)
N2	C10	1.340(4)	Cl5	Sb2	Cl7	91.38(2)
N2	C6	1.339(4)	Cl5	Sb2	Cl8	90.90(2)
N1	C1	1.333(4)	Cl4	Sb1	Cl9	88.91(2)
N1	C5	1.341(3)	Cl3	Sb1	Cl4	93.20(2)
Cl2	Sb2	3.0148(8)	Cl3	Sb1	Cl9	174.51(2)
C9	C10	1.377(4)	Cl2	Sb2	Cl5	82.59(2)
C8	C9	1.384(4)	Cl2	Sb2	Cl6	93.48(2)
C7	C8	1.378(4)	Cl2	Sb2	Cl7	91.98(2)
C6	C7	1.378(4)	Cl2	Sb2	Cl8	173.48(2)
C4	C5	1.376(4)	Cl2	Sb1	Cl3	90.02(2)
C3	C4	1.386(4)	Cl2	Sb1	Cl4	175.92(2)
C2	C3	1.389(3)	Cl2	Sb1	Cl9	87.66(2)
C14	C15	1.365(5)	Cl1	Sb1	Cl2	89.01(2)
C13	C14	1.373(4)	Cl1	Sb1	Cl3	90.17(2)
C12	C13	1.374(4)	Cl1	Sb1	Cl4	88.48(2)
C11	C12	1.367(5)	Cl1	Sb1	Cl9	84.82(2)
C1	C2	1.377(4)	C8	C9	C10	117.8(2)
Br3A	C13	1.88(1)	C7	C8	C9	121.4(2)
Br2	C8	1.880(2)	C6	N2	C10	122.6(2)
Br1	C3	1.873(3)	C6	C7	C8	118.3(2)
			C3	C4	C5	118.7(2)
			C2	C3	C4	120.5(2)
			C13	C14	C15	118.3(3)
			C12	C13	C14	120.8(3)
			C11	N3	C15	122.5(3)
			C11	C12	C13	118.5(3)
			C1	N1	C5	122.9(2)
			C1	C2	C3	118.2(2)
			Br3A	C13	C12	109.0(3)
			Br3A	C13	C14	129.8(3)
			Br2	C8	C7	118.8(2)
			Br2	C8	C9	119.8(2)
			Br1	C3	C2	120.2(2)
			Br1	C3	C4	119.3(2)

Figure S4. ORTEP drawing of compound **4**, $(C_5H_6N)[SbBr_4]$.

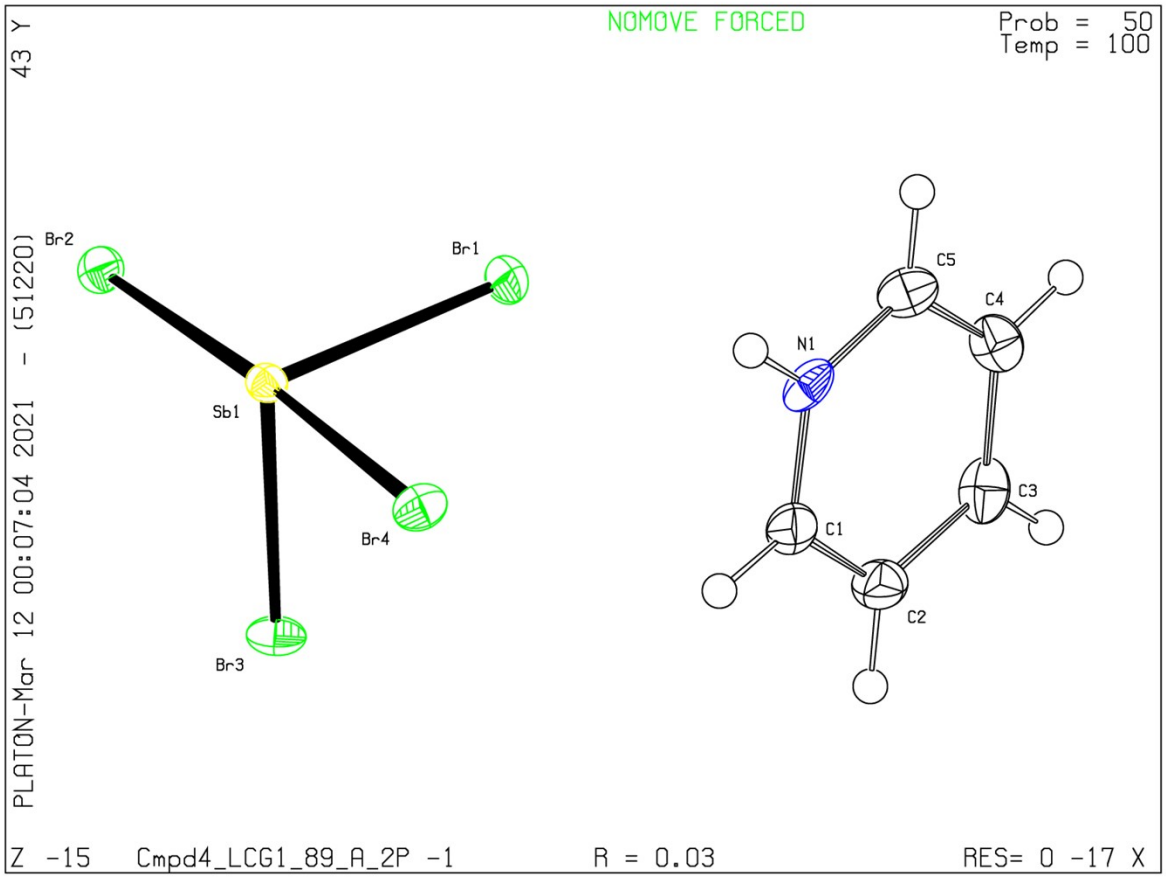

Table S4. Bond distances and angles for compound **4**, $(C_5H_6N)[SbBr_4]$.

Atom1	Atom2	Length (Å)	Atom1	Atom2	Atom3	Angle (°)
Sb1	Br1	2.5778(7)	Sb1	Br2	Sb1	91.31(1)
Sb1	Br1	2.5778(7)	Sb1	Br2	Sb1	91.31(1)
Sb1	Br2	2.9502(8)	C4	C5	N1	119.1(4)
Sb1	Br2	2.9502(8)	C3	C4	C5	119.8(4)
Sb1	Br2	3.1036(8)	C2	C3	C4	118.8(5)
Sb1	Br3	2.5569(7)	C2	C1	N1	119.1(4)
Sb1	Br3	2.5569(7)	C1	N1	C5	123.5(4)
Sb1	Br4	2.6995(8)	C1	C2	C3	119.6(5)
Sb1	Br4	2.6995(8)	Br4	Sb1	Br2	91.20(1)
C5	N1	1.331(6)	Br3	Sb1	Br2	86.96(2)
C4	C5	1.377(7)	Br3	Sb1	Br4	88.91(2)
C3	C4	1.380(7)	Br3	Sb1	Br4	88.91(2)
C2	C3	1.400(7)	Br2	Sb1	Br1	175.45(2)
C1	C2	1.365(7)	Br2	Sb1	Br2	88.69(1)
C1	N1	1.339(6)	Br2	Sb1	Br2	88.69(1)
Br2	Sb1	3.1036(8)	Br2	Sb1	Br3	86.59(2)
			Br2	Sb1	Br3	86.59(2)
			Br2	Sb1	Br3	86.96(2)
			Br2	Sb1	Br4	175.49(2)
			Br2	Sb1	Br4	175.49(2)
			Br2	Sb1	Br4	91.20(1)
			Br1	Sb1	Br2	175.45(2)
			Br1	Sb1	Br2	87.16(2)
			Br1	Sb1	Br2	87.16(2)
			Br1	Sb1	Br3	94.66(2)
			Br1	Sb1	Br3	94.66(2)
			Br1	Sb1	Br4	93.08(2)
			Br1	Sb1	Br4	93.08(2)

Figure S5. ORTEP drawing of compound **5**, $(C_5H_5NCl)[SbBr_4]$.

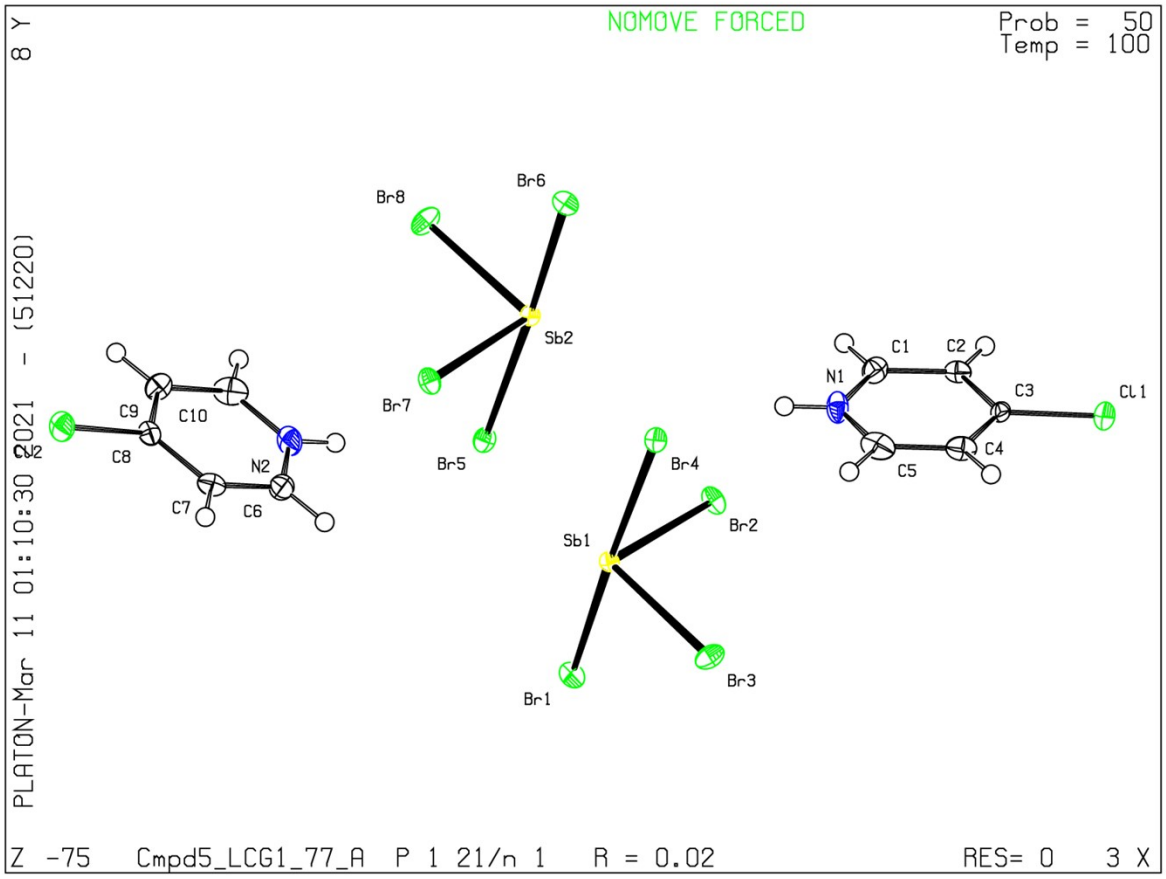

Table S5. Bond distances and angles for compound **5**, $(C_5H_5NCl)[SbBr_4]$.

Atom1	Atom2	Length (Å)	Atom1	Atom2	Atom3	Angle (°)
N2	C6	1.328(5)	C1	C2	C3	118.2(3)
C1	N1	1.344(5)	C3	C4	C5	118.2(3)
N1	C5	1.344(5)	C8	C7	C6	118.3(3)
N2	C10	1.345(5)	C8	C9	C10	118.4(3)
C1	C2	1.369(5)	Cl1	C3	C2	118.9(3)
C7	C6	1.371(5)	Cl2	C8	C7	119.5(3)
C9	C10	1.374(6)	N1	C5	C4	119.6(3)
C4	C5	1.376(6)	N2	C10	C9	119.7(3)
C8	C9	1.378(5)	Cl1	C3	C4	119.8(3)
C3	C4	1.383(5)	Cl2	C8	C9	119.8(3)
C2	C3	1.385(5)	N1	C1	C2	119.9(3)
C7	C8	1.396(5)	N2	C6	C7	119.9(3)
Cl2	C8	1.717(4)	C7	C8	C9	120.7(3)
Cl1	C3	1.720(3)	C2	C3	C4	121.3(3)
Sb1	Br2	2.5475(6)	C1	N1	C5	122.8(3)
Sb2	Br7	2.5580(6)	C10	N2	C6	122.9(3)
Sb1	Br3	2.5841(7)	Br4	Sb2	Br8	173.89(2)
Sb2	Br8	2.5941(7)	Br3	Sb1	Br5	174.39(2)
Sb2	Br6	2.6758(4)	Br1	Sb1	Br4	177.50(2)
Sb1	Br1	2.7282(5)	Br5	Sb2	Br6	177.99(2)
Sb1	Br4	2.9045(4)	Br4	Sb2	Br7	85.89(2)
Sb2	Br5	2.9884(5)	Br3	Sb1	Br4	86.23(2)
Sb1	Br5	3.1170(7)	Br5	Sb2	Br8	86.65(2)
Sb2	Br4	3.1229(7)	Br5	Sb1	Br2	87.30(2)
			Br4	Sb2	Br5	87.57(1)
			Br4	Sb1	Br2	88.00(2)
			Br5	Sb2	Br7	88.72(2)
			Br4	Sb1	Br5	89.18(1)
			Br1	Sb1	Br2	89.65(2)
			Br6	Sb2	Br7	89.92(2)
			Sb1	Br5	Sb2	90.88(1)
			Br1	Sb1	Br5	91.57(2)
			Br6	Sb2	Br8	92.01(2)
			Sb1	Br4	Sb2	92.35(1)
			Br1	Sb1	Br3	93.15(2)
			Br4	Sb2	Br6	93.81(2)
			Br3	Sb1	Br2	95.74(2)
			Br7	Sb2	Br8	95.97(2)

Figure S6. ORTEP drawing of compound **6**, $(C_5H_6N)[SbI_4]$.

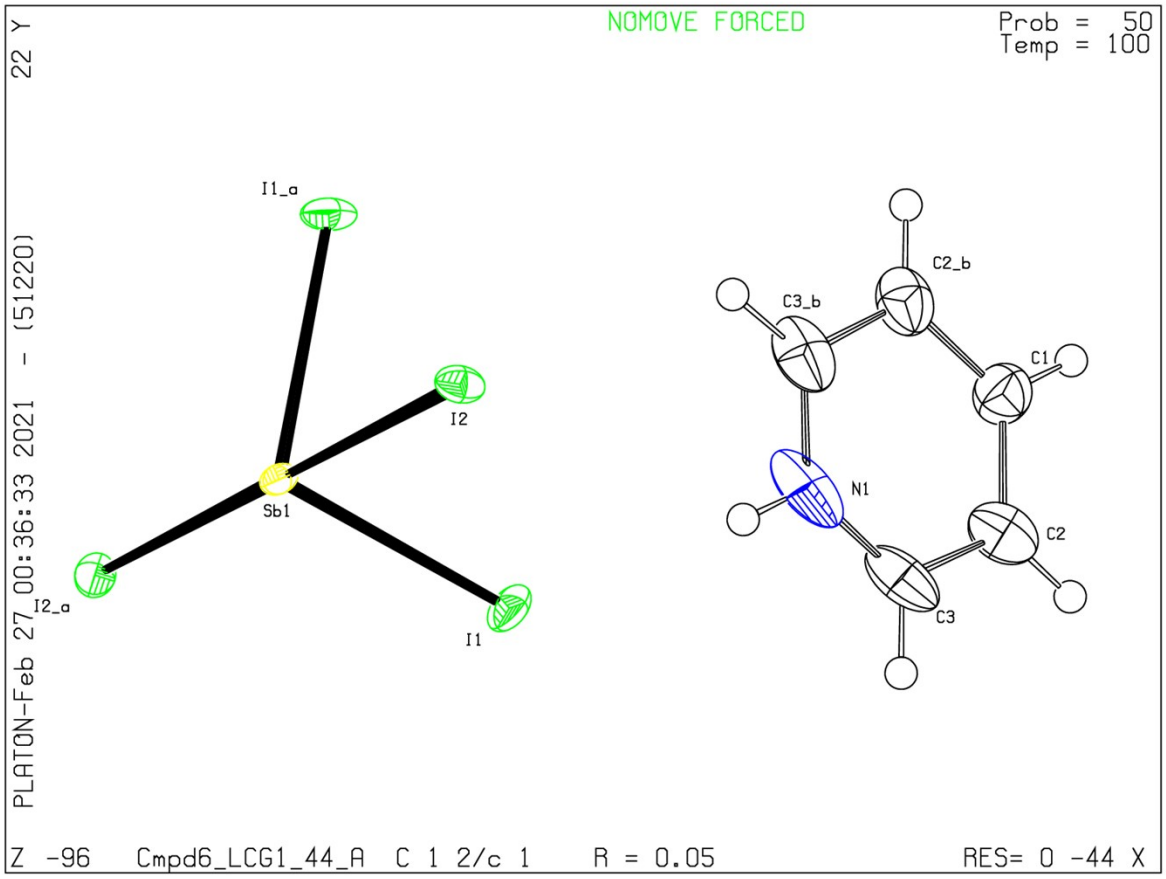

Table S6. Bond distances and angles for compound **6**, $(C_5H_6N)[SbI_4]$.

Atom1	Atom2	Length (Å)	Atom1	Atom2	Atom3	Angle (°)
I1	Sb1	2.8313(15)	I1	Sb1	I1	93.76(6)
I2	Sb1	3.0630(13)	I1	Sb1	I2	92.42(4)
N1	C3	1.33(2)	I1	Sb1	I2	88.02(3)
C1	C2	1.38(2)	I1	Sb1	I2	88.02(3)
C2	C3	1.40(3)	I1	Sb1	I2	92.42(4)
			I2	Sb1	I2	179.36(6)
			C3	N1	C3	123.(2)
			C2	C1	C2	122.(2)
			C1	C2	C3	117.6(18)
			N1	C3	C2	120.0(18)

Figure S7. ORTEP drawing of compound **7**, $(C_5H_5NCl)[SbI_4]$.

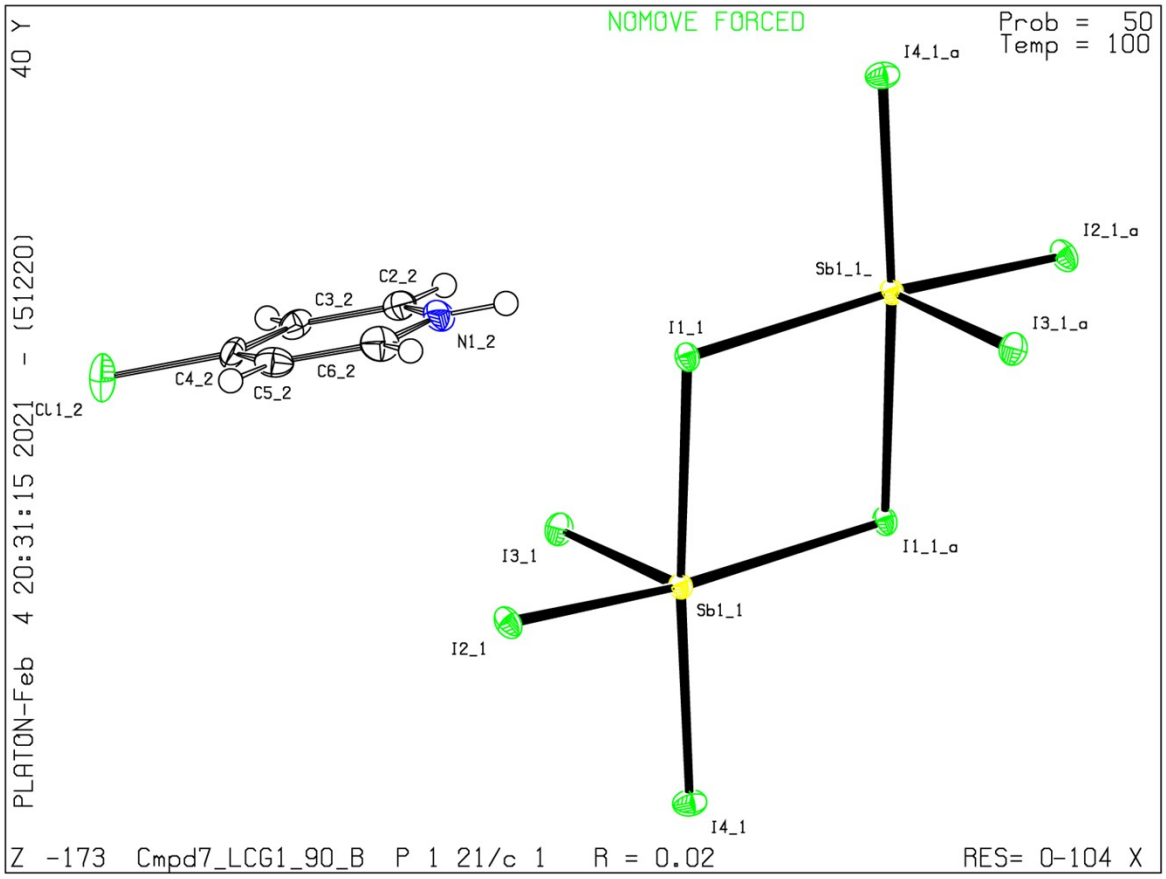

Table S7. Bond distances and angles for compound **7**, $(C_5H_5NCl)[SbI_4]$.

Atom1	Atom2	Length (Å)	Atom1	Atom2	Atom3	Angle (°)
Sb1	I1	3.1835(4)	Sb1	I14	Sb1	92.24(1)
Sb1	I1	3.1835(4)	Sb1	I14	Sb1	92.24(1)
Sb1	I1	3.1955(4)	Sb1	I1	Sb1	93.30(1)
Sb1	I2	2.8540(4)	Sb1	I1	Sb1	93.30(1)
Sb1	I3	2.8205(6)	N1	C6	C5	119.7(3)
Sb1	I4	2.9080(4)	N1	C2	C3	120.2(3)
Sb1	I4	2.9080(4)	I3	Sb1	I1	88.45(1)
Sb1	I4	3.3775(6)	I3	Sb1	I14	169.86(1)
N1	C2	1.346(5)	I3	Sb1	I14	91.23(1)
N1	C6	1.343(5)	I2	Sb1	I1	171.59(1)
I4	Sb1	3.3775(6)	I2	Sb1	I14	93.82(1)
I1	Sb1	3.1955(4)	I2	Sb1	I14	94.05(1)
Cl1	C4	1.716(4)	I2	Sb1	I3	96.08(1)
C5	C6	1.381(5)	I14	Sb1	I1	93.15(1)
C4	C5	1.388(5)	I14	Sb1	I14	87.76(1)
C3	C4	1.390(5)	I14	Sb1	I14	87.76(1)
C2	C3	1.370(5)	I1	Sb1	I1	86.70(1)
			I1	Sb1	I1	86.70(1)
			I1	Sb1	I14	173.51(1)
			I1	Sb1	I14	81.54(1)
			I1	Sb1	I14	85.79(1)
			I1	Sb1	I2	85.84(1)
			I1	Sb1	I3	95.25(1)
			Cl1	C4	C3	119.7(3)
			Cl1	C4	C5	119.0(3)
			C4	C5	C6	118.1(3)
			C3	C4	C5	121.3(3)
			C2	N1	C6	122.6(3)
			C2	C3	C4	118.0(3)

Figure S8. ORTEP drawing of compound **8**, $(C_5H_5NBr)[SbI_4]$.

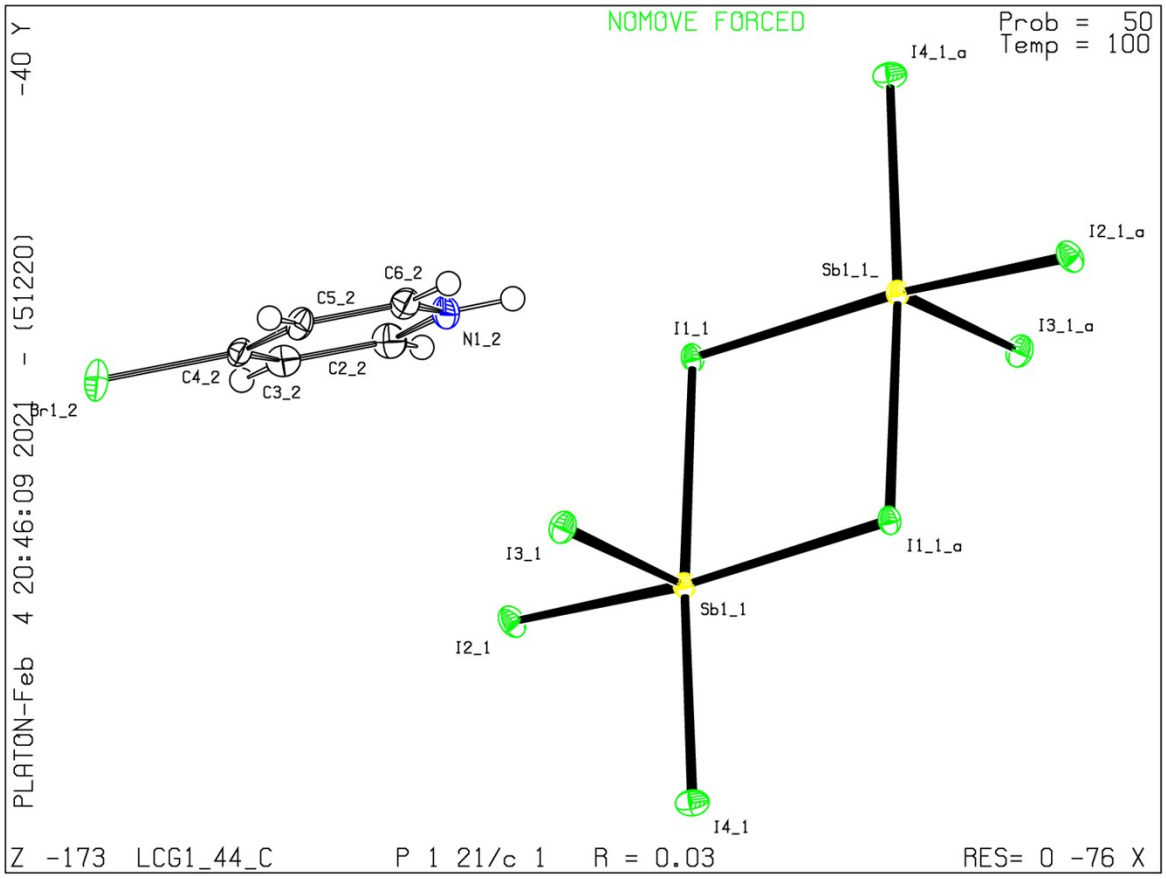

Table S8. Bond distances and angles for compound **8**, $(C_5H_5NBr)[SbI_4]$.

Atom1	Atom2	Length (Å)	Atom1	Atom2	Atom3	Angle (°)
Sb1	I1	3.1660(4)	Sb1	I4	Sb1	92.78(1)
Sb1	I2	2.8487(4)	Sb1	I4	Sb1	92.78(1)
Sb1	I3	2.8183(6)	Sb1	I1	Sb1	93.19(1)
Sb1	I4	2.9232(3)	Sb1	I1	Sb1	93.19(1)
N1	C2	1.340(5)	N1	C6	C5	119.5(3)
N1	C6	1.346(4)	N1	C2	C3	119.7(3)
C5	C6	1.381(4)	I4	Sb1	I1	93.03(1)
C4	C5	1.393(4)	I4	Sb1	I4	87.22(1)
C3	C4	1.387(4)	I4	Sb1	I4	87.22(1)
C2	C3	1.383(4)	I3	Sb1	I1	88.30(1)
Br1	C4	1.873(3)	I3	Sb1	I4	168.93(1)
			I3	Sb1	I4	91.10(1)
			I2	Sb1	I1	171.91(1)
			I2	Sb1	I3	95.95(1)
			I2	Sb1	I4	93.76(1)
			I2	Sb1	I4	95.08(1)
			I1	Sb1	I1	86.81(1)
			I1	Sb1	I1	86.81(1)
			I1	Sb1	I2	85.94(1)
			I1	Sb1	I3	95.37(1)
			I1	Sb1	I4	173.52(1)
			I1	Sb1	I4	80.87(1)
			I1	Sb1	I4	86.36(1)
			C4	C5	C6	118.1(3)
			C3	C4	C5	121.4(3)
			C2	N1	C6	123.4(3)
			C2	C3	C4	118.1(3)
			Br1	C4	C3	118.6(2)
			Br1	C4	C5	120.0(2)

Figure S9. ESP surfaces of *para*-halopyridinium cations used in the synthesis of **1-8**.

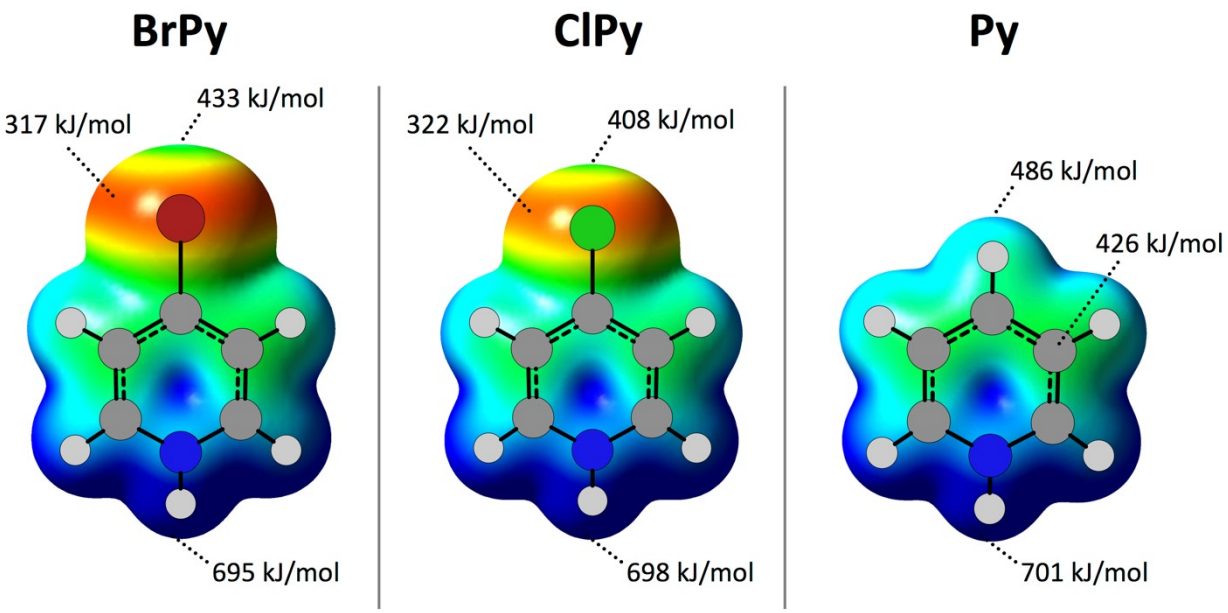

Figure S10. Tauc plot of compounds **1-8**.

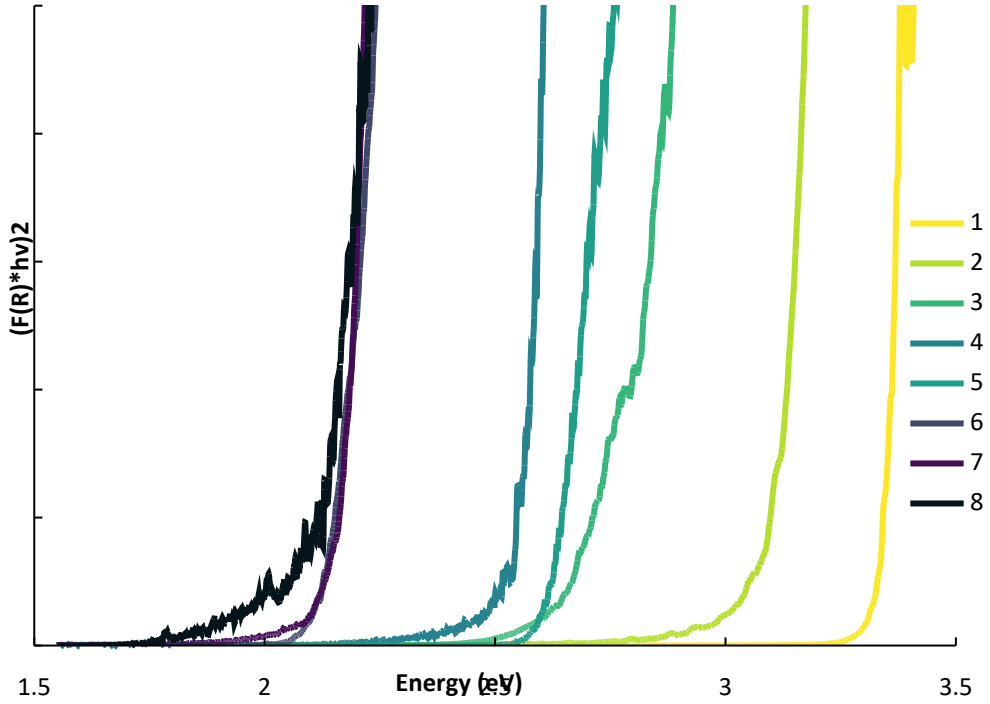

Figure S11. NBO calculation models of **1-8**.

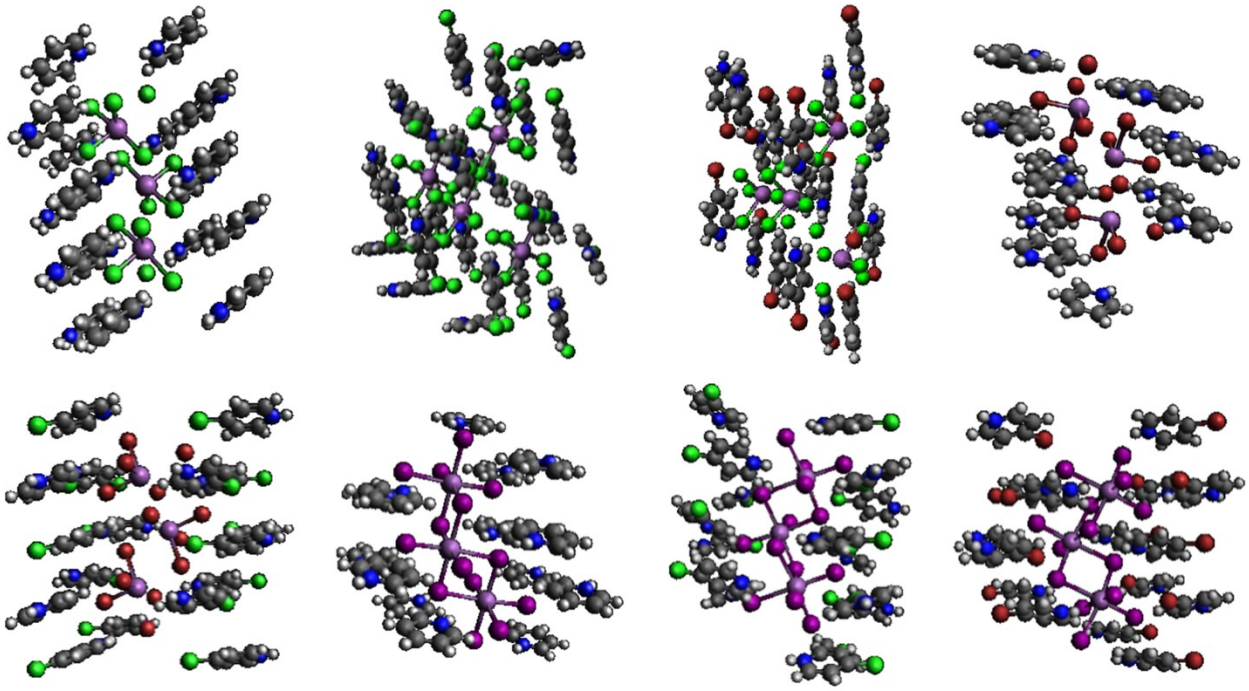

Table S9. NLMO metrics for specific atoms in SbX bond

			Halide			Metal	
	Sb-X	Cation	Halide Cont.	%s-Orbital	%p-Orbital	Metal Cont.	%p-Orbital
1	Sb1-Cl3	HPy	78.163	19.35	80.17	20.491	94.1
1	Sb1-Cl4	HPy	80.137	20.55	79.02	18.247	96.42
1	Sb1-Cl5	HPy	83.933	19.48	80.26	15.087	97.75
1	Sb1-Cl2	HPy	89.764	17.48	82.46	8.366	98.11
1	Sb1-Cl16	HPy	94.984	4.87	95.1	3.329	97.11
1	Sb1-Cl7	HPy	95.625	16.36	83.59	2.705	96.37
2	Sb1-Cl4	ClPy	79.397	20.5	79.09	19.192	94.67
2	Sb1-Cl2	ClPy	81.606	20.27	79.35	17.173	96.9
2	Sb1-Cl5	ClPy	81.982	20.55	79.12	16.578	97.06
2	Sb1-Cl7	ClPy	91.543	1.38	98.62	4.612	97.87
2	Sb1-Cl6	ClPy	91.409	0.67	99.33	4.597	97.74
2	Sb1-Cl15	ClPy	91.811	1.27	97.09	3.122	97.11
3	Sb1-Cl2	BrPy	79.038	19.09	80.41	19.636	94.91
3	Sb1-Cl4	BrPy	80.39	19.8	79.87	18.189	95.7
3	Sb1-Cl5	BrPy	84.372	21.21	78.55	14.734	97.93
3	Sb1-Cl3	BrPy	88.647	5.74	94.23	7.811	97.94
3	Sb1-Cl11	BrPy	91.25	3.49	96.5	5.605	97.76
3	Sb1-Cl16	BrPy	97.667	66.6	33.4	1.291	96.66
4	Sb7-Br8	HPy	74.623	16.31	83.27	22.866	96.32
4	Sb7-Br10	HPy	77.034	18.2	81.44	20.509	97.96
4	Sb7-Br9	HPy	81.45	16.07	83.73	17.246	97.96
4	Sb7-Br11	HPy	86.459	16.39	83.48	11.054	98.06
4	Sb7-Br6	HPy	92.583	1.19	98.75	3.981	96.97
4	Sb7-Br14	HPy	94.289	14.73	85.22	3.669	96.33
5	Sb3-Br8	ClPy	74.784	16.58	82.99	23.157	95.9
5	Sb3-Br9	ClPy	78.32	18.67	81	19.832	97.84
5	Sb3-Br7	ClPy	81.058	18.05	81.73	17.772	98.37
5	Sb3-Br6	ClPy	86.776	16.46	83.42	10.062	98.16
5	Sb3-Br5	ClPy	92.231	2.89	97.03	4.766	97.26
5	Sb3-Br12	ClPy	94.096	13.24	86.7	3.62	96.09
6	Sb1-I5	HPy	72.83	14.47	85.23	26.875	97.94
6	Sb1-I7	HPy	72.832	14.47	85.23	26.873	97.97
6	Sb1-I6	HPy	80.768	13.2	86.64	17.839	98.63
6	Sb1-I4	HPy	80.749	13.21	86.64	17.859	98.63
6	Sb1-I9	HPy	89.519	10.58	89.36	7.195	96.87
6	Sb1-I8	HPy	89.524	10.55	89.39	7.19	96.87
7	Sb3-I5	ClPy	70.612	13.13	86.49	29.027	97.72
7	Sb3-I6	ClPy	75.608	15.76	84.05	24.041	98.59
7	Sb3-I4	ClPy	76.506	13.6	86.19	22.998	98.86
7	Sb3-I7	ClPy	84.098	15.03	84.87	11.815	97.78
7	Sb3-I8	ClPy	86.162	11.23	88.64	9.871	97.8
7	Sb3-I9	ClPy	91.479	7.33	92.63	5.312	96.23
8	Sb1-I4	BrPy	71.697	13.65	86.03	27.946	97.96
8	Sb1-I5	BrPy	74.294	14.88	84.87	25.398	98.45
8	Sb1-I6	BrPy	74.772	13.33	86.42	24.822	98.83
8	Sb1-I7	BrPy	85.095	14.99	84.9	10.635	97.63
8	Sb1-I9	BrPy	87.857	23.42	76.54	7.668	97.28
8	Sb1-I8	BrPy	90.188	9.88	90.02	6.215	96.78

Table S10. Specific SOPT values for NCI stabilization energy (kcal/mol).

				Stabilization Energy (kCal/mol)				
#	**Metal-Halide**	**Cation**	**Atom**	**X-X**	**X-H**	**X-C**	**X-π**	**Total**
1	SbCl	HPy	Sb1-Cl2	0.00	6.04	0.45	1.03	7.52
1	SbCl	HPy	Sb1-Cl3	0.00	1.09	0.17	0.83	2.09
1	SbCl	HPy	Sb1-Cl4	0.00	1.53	0.19	0.49	2.21
1	SbCl	HPy	Sb1-Cl5	0.00	1.55	0.52	0.13	2.20
1	SbCl	HPy	Sb1-Cl16	0.00	1.52	0.53	0.07	2.12
1	SbCl	HPy	Sb1-Cl7	0.00	6.86	0.39	1.26	8.51
2	SbCl	ClPy	Sb1-Cl2	0.00	1.13	0.23	0.51	1.87
2	SbCl	ClPy	Sb1-Cl4	0.00	1.39	0.18	0.24	1.81
2	SbCl	ClPy	Sb1-Cl5	0.07	1.17	0.00	0.81	2.05
2	SbCl	ClPy	Sb1-Cl6	1.57	9.29	0.27	0.38	11.51
2	SbCl	ClPy	Sb1-Cl7	0.00	5.00	0.28	0.23	5.51
2	SbCl	ClPy	Sb1-Cl15	0.00	4.52	0.29	0.20	5.01
3	SbCl	BrPy	Sb1-Cl4	2.59	0.59	0.42	0.13	3.73
3	SbCl	BrPy	Sb1-Cl5	0.00	3.89	0.61	0.34	4.84
3	SbCl	BrPy	Sb1-Cl2	0.00	1.01	0.31	0.83	2.15
3	SbCl	BrPy	Sb1-Cl3	0.00	3.51	0.21	0.64	4.36
3	SbCl	BrPy	Sb1-Cl11	0.00	6.61	0.28	1.16	8.05
3	SbCl	BrPy	Sb1-Cl16	0.00	2.40	0.27	0.20	2.87
4	SbBr	HPy	Sb7-Br6	0.00	2.80	0.77	0.10	3.67
4	SbBr	HPy	Sb7-Br8	0.00	0.85	0.23	0.66	1.74
4	SbBr	HPy	Sb7-Br9	0.00	0.85	0.19	0.12	1.16
4	SbBr	HPy	Sb7-Br10	0.00	0.50	0.24	1.20	1.94
4	SbBr	HPy	Sb7-Br11	0.00	2.74	0.74	0.18	3.66
4	SbBr	HPy	Sb7-Br14	0.00	0.94	0.21	0.20	1.35
5	SbBr	ClPy	Sb3-Br5	0.29	5.42	0.44	0.00	6.15
5	SbBr	ClPy	Sb3-Br6	0.00	7.31	0.20	0.00	7.51
5	SbBr	ClPy	Sb3-Br7	0.00	2.54	0.00	0.60	3.14
5	SbBr	ClPy	Sb3-Br8	1.67	0.15	0.00	1.60	3.42
5	SbBr	ClPy	Sb3-Br9	0.05	0.33	0.18	1.18	1.74
5	SbBr	ClPy	Sb3-Br12	0.00	1.25	0.21	0.08	1.54
6	SbI	HPy	Sb1-I4	0.00	1.62	0.27	0.26	2.15
6	SbI	HPy	Sb1-I5	0.00	0.72	0.22	1.07	2.01
6	SbI	HPy	Sb1-I6	0.00	1.62	0.27	0.26	2.15
6	SbI	HPy	Sb1-I7	0.00	0.72	0.22	1.07	2.01
6	SbI	HPy	Sb1-I8	0.00	1.84	0.31	0.16	2.31
6	SbI	HPy	Sb1-I9	0.00	1.85	0.31	0.16	2.32
7	SbI	ClPy	Sb3-I4	0.32	1.00	0.06	0.05	1.43
7	SbI	ClPy	Sb3-I5	0.66	1.41	0.05	0.80	2.92
7	SbI	ClPy	Sb3-I6	0.00	2.25	0.51	0.96	3.72
7	SbI	ClPy	Sb3-I7	0.00	3.42	0.76	0.46	4.64
7	SbI	ClPy	Sb3-I8	0.31	0.93	0.10	0.00	1.34
7	SbI	ClPy	Sb3-I9	0.00	3.76	0.83	0.50	5.09
8	SbI	BrPy	Sb1-I4	0.14	1.03	0.34	1.30	2.81
8	SbI	BrPy	Sb1-I5	0.00	1.98	0.11	1.99	4.08
8	SbI	BrPy	Sb1-I6	2.01	0.54	0.05	0.31	2.91
8	SbI	BrPy	Sb1-I7	0.18	4.95	0.89	0.00	6.02
8	SbI	BrPy	Sb1-I8	2.05	0.52	0.07	0.40	3.04
8	SbI	BrPy	Sb1-I9	0.27	5.65	0.91	0.00	6.83

Table S11. QTAIM metrics for the three crystallographically unique Sb-X bonds in **1-8**.

Compound	Metal-Halide	Cation	WBI	e^- Density	Laplacian
1	SbCl	HPy	0.3141	0.03831923	0.0581074
1	SbCl	HPy	0.6765	0.08620254	0.1196433
1	SbCl	HPy	0.6409	0.08318599	0.11902492
1	SbCl	HPy	0.4904	0.06641973	0.09215661
1	SbCl	HPy	0.1105	0.02326767	0.04621105
1	SbCl	HPy	0.1509	0.0204002	0.04424879
2	SbCl	ClPy	0.5874	0.07764108	0.10890344
2	SbCl	ClPy	0.6156	0.08345464	0.11907223
2	SbCl	ClPy	0.5683	0.07632051	0.10793928
2	SbCl	ClPy	0.2031	0.02642162	0.04778619
2	SbCl	ClPy	0.2108	0.0288469	0.05223379
2	SbCl	ClPy	0.1716	0.02322426	0.0451892
3	SbCl	BrPy	0.5818	0.08505781	0.11473975
3	SbCl	BrPy	0.4854	0.04152379	0.06224566
3	SbCl	BrPy	0.6734	0.07896259	0.11261854
3	SbCl	BrPy	0.3201	0.06687976	0.09507381
3	SbCl	BrPy	0.2345	0.02882461	0.04926791
3	SbCl	BrPy	0.0877	0.01649106	0.03822917
4	SbBr	HPy	0.2265	0.02605232	0.04006254
4	SbBr	HPy	0.7133	0.07103509	0.06056187
4	SbBr	HPy	0.5127	0.05218683	0.05158904
4	SbBr	HPy	0.6572	0.06856559	0.06595465
4	SbBr	HPy	0.3717	0.03627113	0.04309411
4	SbBr	HPy	0.1428	0.01925834	0.03455599
5	SbBr	ClPy	0.2292	0.02686261	0.04061767
5	SbBr	ClPy	0.3671	0.0349583	0.04199982
5	SbBr	ClPy	0.5244	0.05817985	0.05974371
5	SbBr	ClPy	0.7123	0.07244802	0.06268986
5	SbBr	ClPy	0.6395	0.06706069	0.06530618
5	SbBr	ClPy	0.1446	0.01928907	0.03449916
6	SbI	HPy	0.4872	0.03992645	0.03280466
6	SbI	HPy	0.7093	0.05807797	0.0297083
6	SbI	HPy	0.4877	0.03998232	0.03280626
6	SbI	HPy	0.7093	0.05807809	0.02970983
6	SbI	HPy	0.2678	0.02459406	0.03137598
6	SbI	HPy	0.2679	0.02461612	0.03139774
7	SbI	ClPy	0.5483	0.04750505	0.03410942
7	SbI	ClPy	0.7811	0.05944099	0.02608264
7	SbI	ClPy	0.6093	0.05144898	0.03374065
7	SbI	ClPy	0.4201	0.03453027	0.03310136
7	SbI	ClPy	0.3433	0.02874337	0.03090945
7	SbI	ClPy	0.216	0.02187476	0.03067514
8	SbI	BrPy	0.7475	0.05742676	0.02807747
8	SbI	BrPy	0.6631	0.05407679	0.03205011
8	SbI	BrPy	0.5944	0.04837339	0.03178601
8	SbI	BrPy	0.3806	0.03241009	0.03295307
8	SbI	BrPy	0.2292	0.02229111	0.03000896
8	SbI	BrPy	0.3091	0.02924107	0.03408277

Figure S12. Correlation plots of **1-8** comparing bandgap energy, Wiberg Indexes, electron density (ρ), octahedral distortion, stabilization energy, Sb-X bond covalency, and intermediate band hybridization. Note that covalency is calcualted by the NLMO determined Sb/X contribution ratio and hybridization is calculated from the DOS determined HOMO Sb s-state / halide p-state ratio. Color scheme: SbCl, teal; SbBr, yellow; SbI, red.