Synthesis and structure-dependent optical properties of two new organic-inorganic hybrid antimony(III) chlorides

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Table S1. Hydrogen bonds for compound **1**

D-H···A[a]	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(DHA) (deg)
N1-H1···Cl14	1.00	2.23	3.106(5)	145.5
N2-H2···Cl5#1	1.00	2.16	3.132(5)	163.7
N3-H3···Cl5	1.00	2.33	3.175(5)	141.9
N4-H4···Cl4#2	1.00	2.20	3.096(5)	148.1
N5-H5···Cl4#3	1.00	2.33	3.157(5)	139.5
N6-H6···Cl3#4	1.00	2.50	3.325(5)	139.6
N6-H6···Cl5#4	1.00	2.43	3.174(5)	130.5

[a] Symmetry transformations used to generate equivalent atoms: #1 1-X, 1-Y, 1-Z; #2 +X, -1+Y, +Z; #3 1-X, 1-Y, 2-Z; #4 1+X, +Y, +Z.

Table S2. Hydrogen bonds for compound **2**

D-H···A	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(DHA) (deg)
N1-H1···Cl6	0.98	2.37	3.165(6)	138.0
N2-H2···Cl5	0.98	2.10	3.023(5)	155.9
N3-H3···Cl6	0.98	2.59	3.292(6)	128.3

Table S3. Torsion angles for the organic cations in compounds **1** and **2**

		A−B−C−D	the torsion angle	conformation
compound **1**	Type I	N1−C3−C4−N2	176.2(4)°	*TTTT*
		C3−C4−N2−C6	177.5(5)°	
		C4−N2−C6−C7	171.1(5)°	
		N2−C6−C7−N3	178.1(4)°	
	Type II	N4−C12−C13−N5	179.3(4)°	*TTGT*
		C12−C13−N5−C15	162.6(5)°	
		C13−N5−C15−C16	55.2(7)°	
		N5−C15−C16−N6	168.8(4)°	
compound **2**		N1−C3−C4−N2	149.9(5)°	*TTGG*
		C3−C4−N2−C6	160.3(5)°	
		C4−N2−C6−C7	66.1(7)°	
		N2−C6−C7−N3	70.0(8)°	

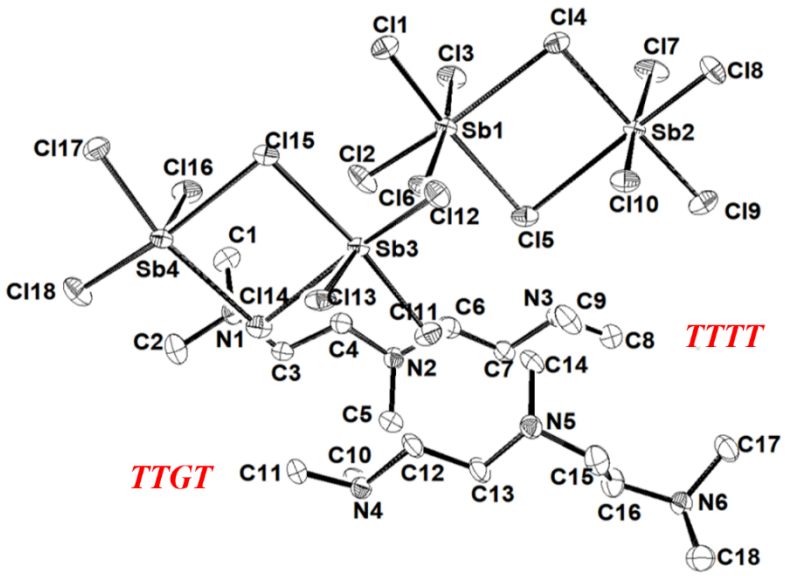

Fig. S1 ORTEP plot of the asymmetric unit of compound **1**, showing the labeling scheme and the 50% probability displacement ellipsoids.

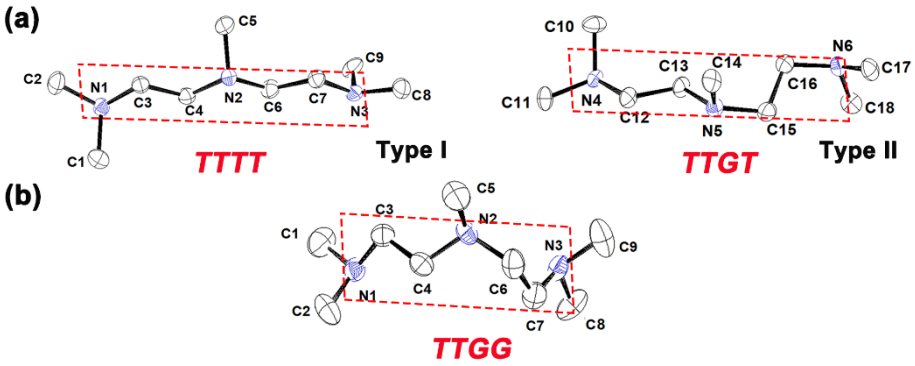

Fig. S2 (a) The *TTTT* conformation of type I organic cation and the *TTGT* conformation of type II organic cation in compound **1**; (b) The *TTGG* conformation of the organic cation in compound **2**.

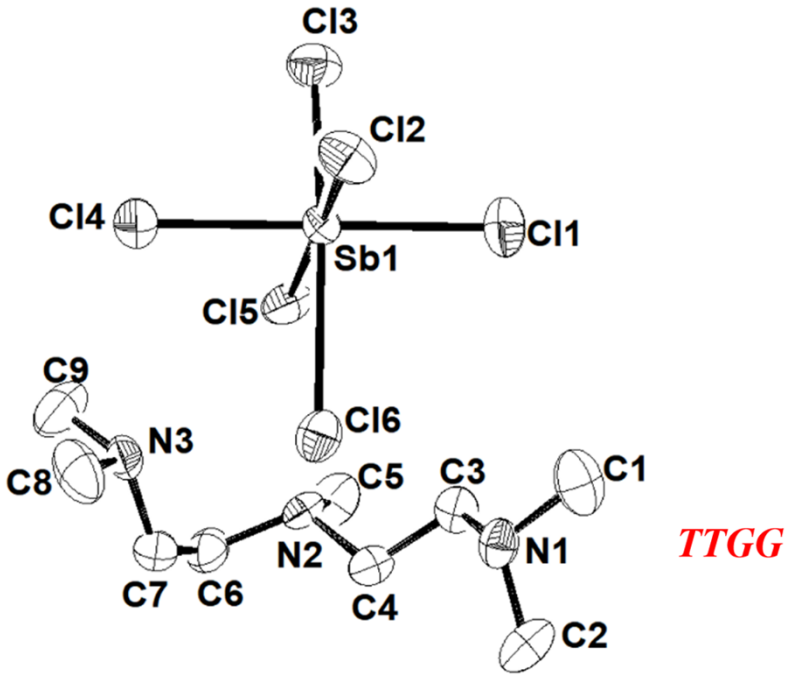

Fig. S3 ORTEP plot of the asymmetric unit of compound **2**, showing the labeling scheme and the 50% probability displacement ellipsoids.

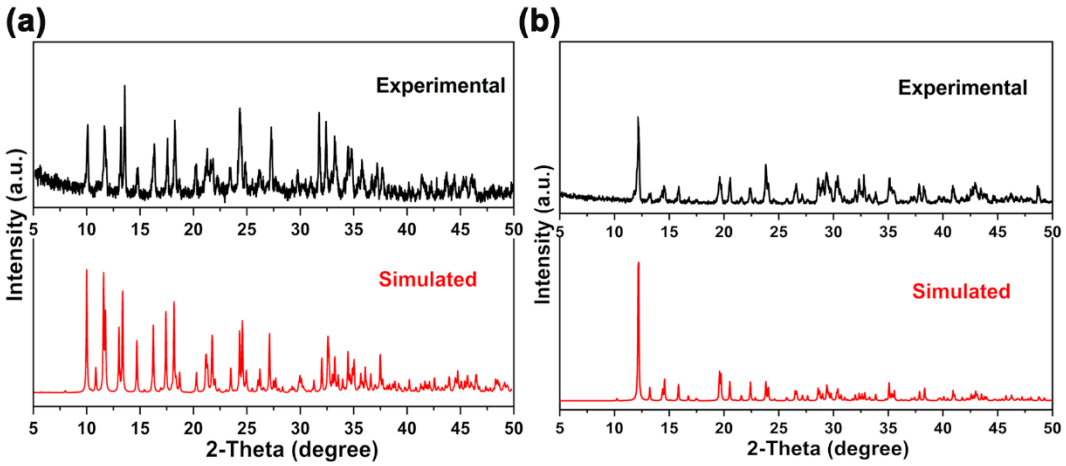

Fig. S4 Experimental and simulated XRD patterns for compound **1** (a) and compound **2** (b).

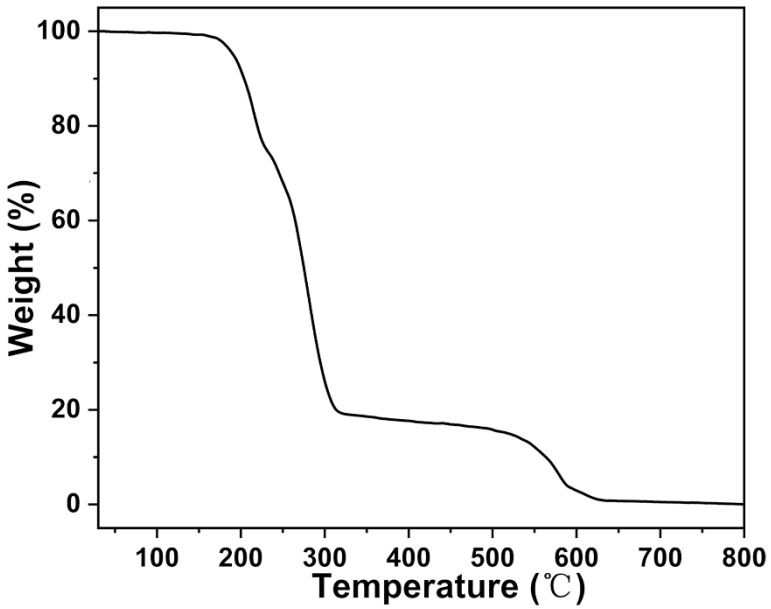

Fig. S5 TGA analysis of compound **1** under N_2 atmosphere.

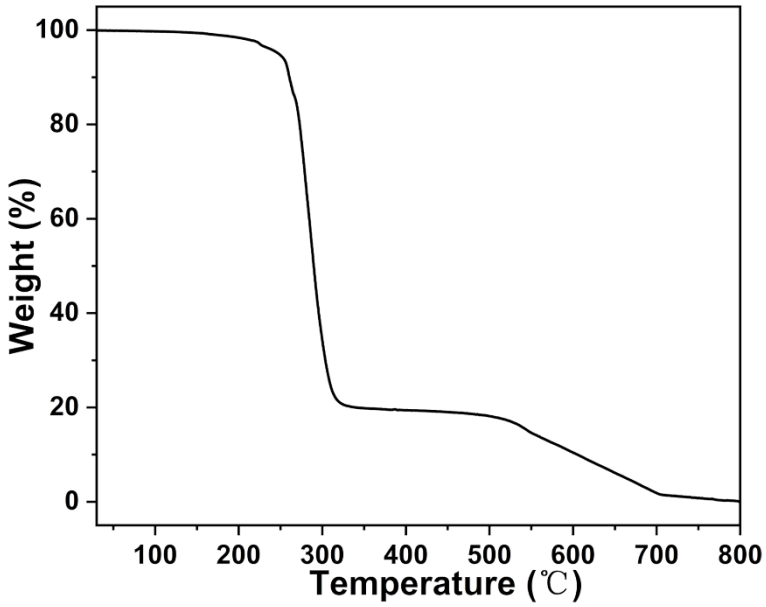

Fig. S6 TGA analysis of compound **2** under N_2 atmosphere.

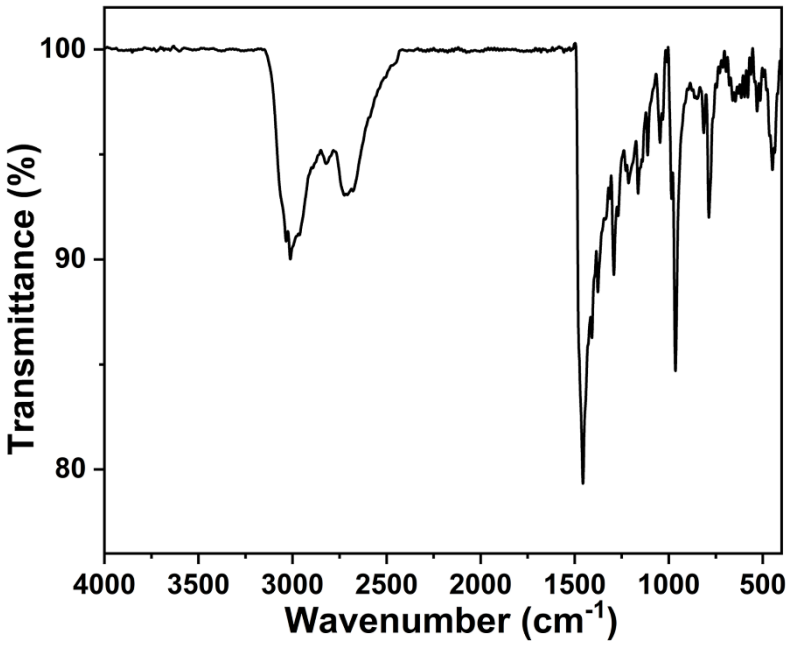

Fig. S7 The IR spectrum of compound **1**.

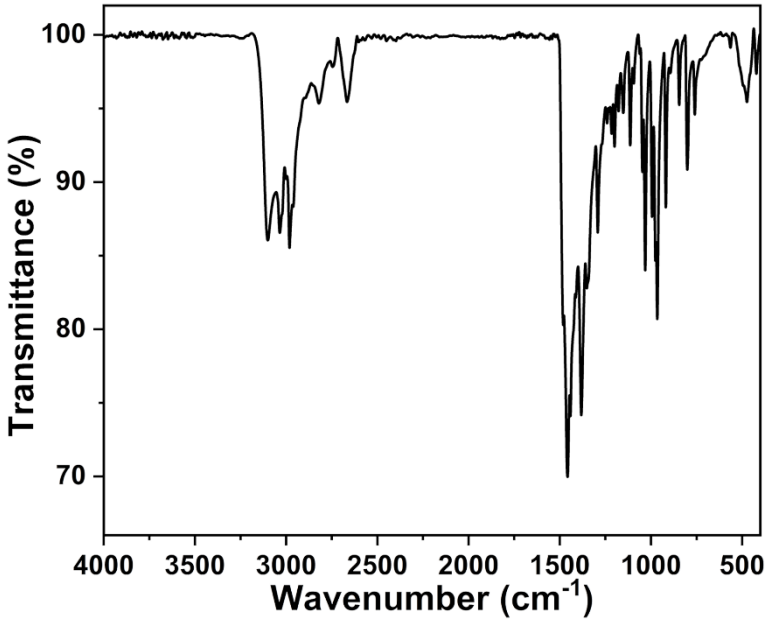

Fig. S8 The IR spectrum of compound **2**.

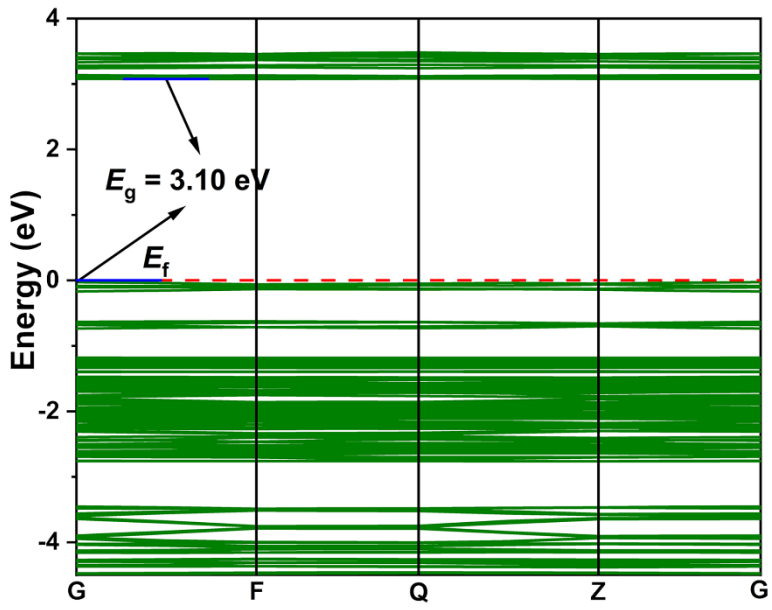

Fig. S9 Calculated band structure of compound **1** (the Fermi level is set at 0 eV).

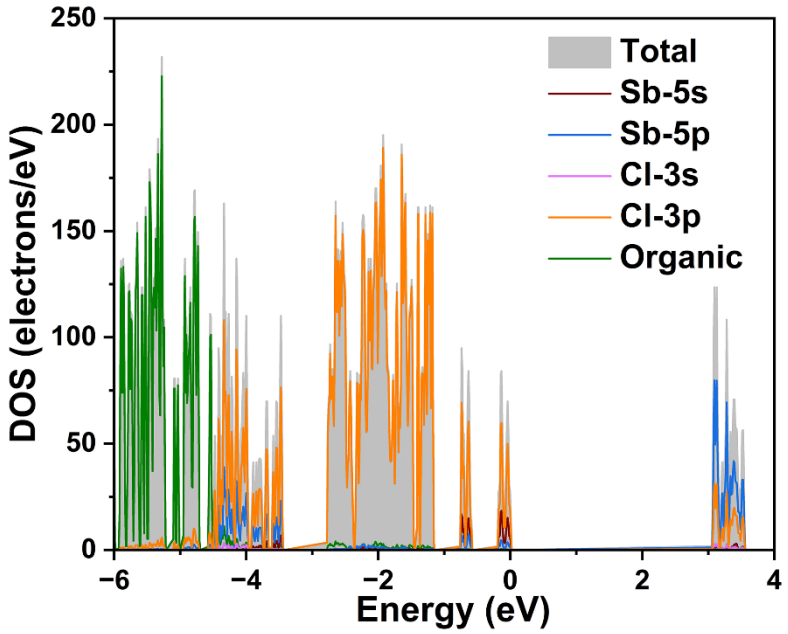

Fig. S10 Total and partial DOSs for compound **1**.

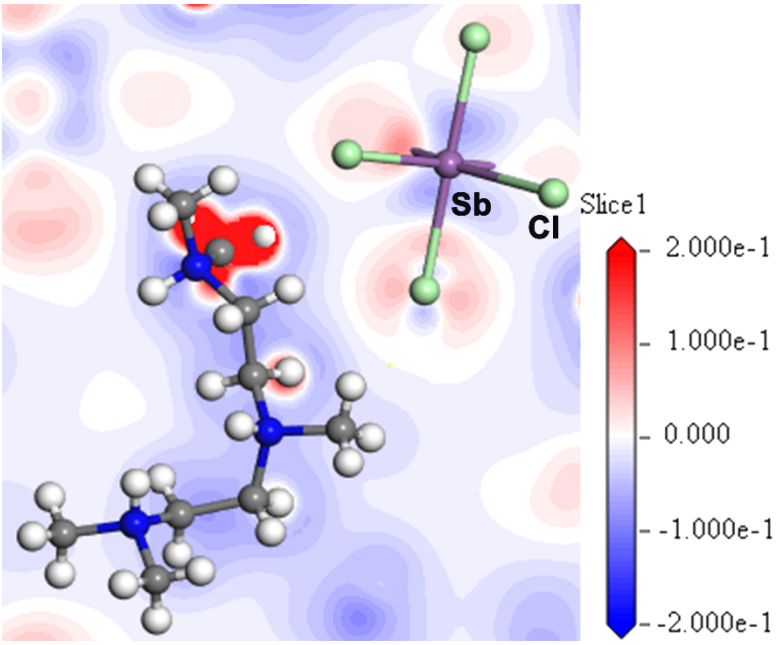

Fig. S11 Electron-density difference map of compound **2**.

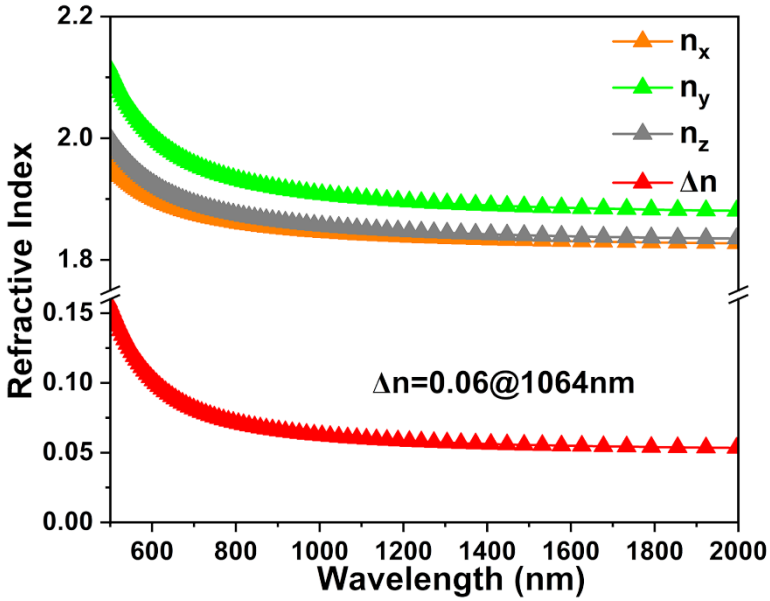

Fig. S12 Calculated dispersion of refractive index curves and birefringence of compound **1**.