Supporting Information

$RbSbSO_4Cl_2$: an excellent sulfate nonlinear optical material generated due to the synergistic effect of three asymmetric chromophores

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Table S1. Atomic coordinates and equivalent isotropic displacement parameters for $RbSbSO_4Cl_2$. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	*x*	*y*	*z*	U_{eq} (Å^2)	BVS
Sb1	0.97056 (11)	0.12441 (8)	0.38528 (4)	0.0082 (2)	2.870
Rb1	0.5207 (2)	0.70373 (12)	0.34032 (6)	0.0157 (3)	0.943
Cl1	0.9061 (4)	−0.0123 (4)	0.24714 (16)	0.0144 (5)	0.861
Cl2	1.0549 (4)	−0.1606 (3)	0.44672 (16)	0.0166 (5)	0.996
S1	0.4948 (4)	0.1887 (3)	0.38712 (14)	0.0087 (5)	5.848
O1	0.6574 (11)	0.0492 (10)	0.4167 (5)	0.0108 (14)	2.101
O2	0.6146 (13)	0.3261 (10)	0.3410 (5)	0.0161 (16)	1.950
O3	0.3828 (13)	0.2614 (12)	0.4610 (5)	0.0187 (17)	1.695
O4	0.3452 (11)	0.0923 (10)	0.3317 (4)	0.0096 (14)	1.972

Table S2. Selected Bond lengths [Å] and angles [°] for $RbSbSO_4Cl_2$.

Sb1—O1	2.123 (7)	O1—Sb1—Cl2	83.3 (2)
Sb1—Cl2	2.382 (3)	O1—Sb1—Cl1	86.7 (2)
Sb1—Cl1	2.438 (3)	Cl2—Sb1—Cl1	91.96 (9)
Sb1—O4^{i}	2.535 (7)	O1—Sb1—O4^{i}	158.7 (3)
Rb1—O2	2.858 (8)	O2—S1—O3	113.1 (5)
Rb1—O1^{iii}	2.956 (8)	O2—S1—O4	112.1 (5)
Rb1—O4^{iv}	2.962 (7)	O3—S1—O4	109.7 (5)
Rb1—O4^{iii}	3.087 (7)	O2—S1—O1	105.6 (4)
Rb1—O2^{iv}	3.121 (9)	O3—S1—O1	109.4 (4)
Rb1—Cl2^{v}	3.383 (3)	O4—S1—O1	106.8 (4)
Rb1—Cl1^{iv}	3.435 (3)	O2—Rb1—O2^{iv}	110.15 (19)
Rb1—Cl1^{iii}	3.544 (3)	O4^{iii}—Rb1—O2^{iv}	65.81 (19)
Rb1—Cl2^{vi}	3.545 (3)	O2—Rb1—Cl2^{v}	83.72 (18)
S1—O2	1.463 (8)	O2—Rb1—O1^{iii}	141.5 (2)
S1—O3	1.468 (8)	O2—Rb1—O4^{iv}	70.8 (2)
S1—O4	1.475 (7)	O1^{iii}—Rb1—O4^{iv}	122.0 (2)
S1—O1	1.532 (8)	O2—Rb1—O4^{iii}	170.6 (2)
Cl2—Sb1—O4^{i}	80.91 (18)	O4^{iv}—Rb1—O4^{iii}	108.83 (17)
Cl1—Sb1—O4^{i}	79.65 (17)		

Symmetry codes: (i) x+1, y, z; (ii) x, y−1, z; (iii) x, y+1, z; (iv) −x+1, y+1/2, −z+1/2; (v) x−1/2, −y+1/2, −z+1; (vi) x−1, y+1, z; (vii) −x+1, y−1/2, −z+1/2; (viii) x+1/2, −y+1/2, −z+1; (ix) x+1, y−1, z; (x) x−1, y, z.

Table S3. Calculation of dipole moments for SO_4, SbO_3Cl_2, RbO_5Cl_4 polyhedra in $RbSbSO_4Cl_2$ (D = Debyes).

$RbSbSO_4Cl_2$				
Polar unit (a unit cell)	Dipole moment (D)			
	x-component	y-component	z-component	total magnitude
SO_4	1.1988974	1.774326	0.093682422	2.143447
	-1.1988974	1.774326	-0.093682422	2.143447
	-1.197792277	-1.77543	0.094428808	2.143772
	-1.199189995	-1.77521	0.095317119	2.144415
	1.199189995	-1.77521	-0.095317119	2.144415
	1.197792277	-1.77543	-0.094428808	2.143772
SbO_3Cl_2	-3.010043015	21.24077434	-0.953131452	21.47415454
	3.00927112	21.24029045	0.955321669	21.47366505
	3.009800592	-21.23967076	-0.955689796	21.47314268
	-3.009555435	-21.24075129	0.952926156	21.47405429
RbO_5Cl_4	-5.271055366	-5.252723139	-1.594764963	7.61041394
	5.270891526	-5.252525211	1.594653489	7.610140493
	5.271019732	5.252674496	-1.594653431	7.610332315
	-5.270891526	5.252525211	1.594653489	7.610140493

Figure S1. The crystal photograph of $RbSbSO_4Cl_2$.

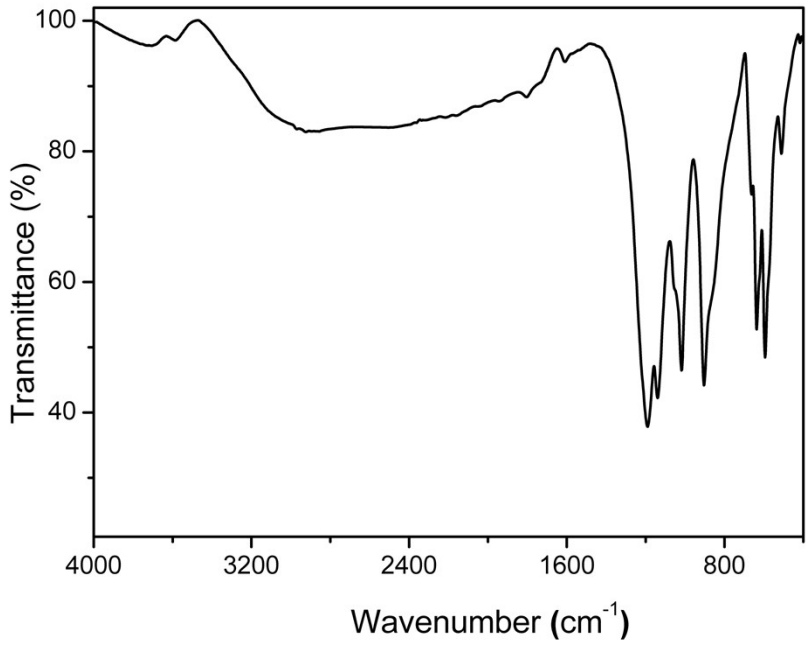

Figure S2. IR spectrum for $RbSbSO_4Cl_2$.

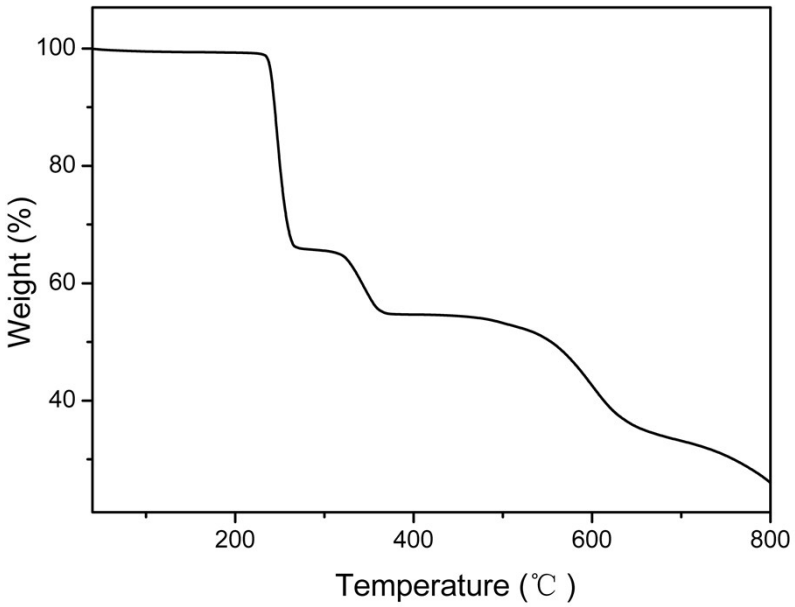

Figure S3. TGA curve for $RbSbSO_4Cl_2$.

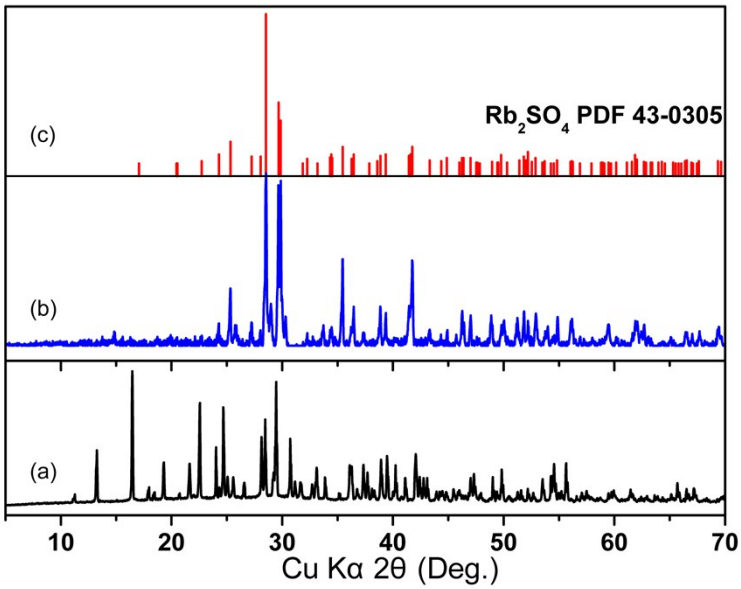

Figure S4. Powder X-ray diffraction (PXRD) patterns for pure phase $RbSbSO_4Cl_2$ (a); the residue for TGA (b); PDF for Rb_2SO_4 (c).

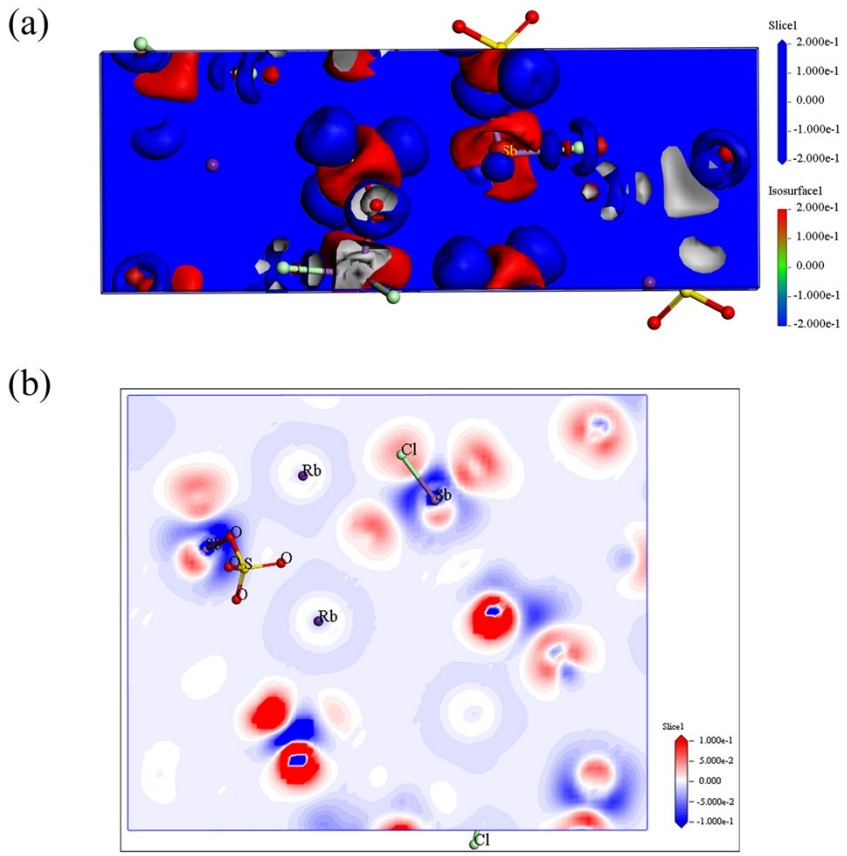

Figure S5. Electron-density difference map for $RbSbSO_4Cl_2$.