Supporting Information

$Rb_3SbF_3(NO_3)_3$: An Excellent Antimony Nitrate Nonlinear Optical Material with Strong Second Harmonic Generation Response Fabricated by a Rationally Multi-component Design

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Table S1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2$ $x10^3$) , and calculated Bond Valence Sum for $Rb_3SbF_3(NO_3)_3$. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	x	y	z	U $_{eq}$ ($Å^2$)	BVS
Sb(1)	3540(1)	4750(1)	6357(1)	22(1)	2.802
Rb(1)	775(1)	3244(1)	9032(1)	25(1)	1.095
Rb(2)	1376(1)	249(1)	4745(1)	25(1)	1.249
Rb(3)	5427(1)	710(1)	8842(1)	27(1)	1.150
N(1)	1846(10)	5317(12)	3091(9)	25(2)	4.784
N(2)	1824(10)	8186(13)	8164(9)	28(2)	4.927
N(3)	6988(10)	5777(13)	8174(9)	25(2)	4.854
F(1)	1532(7)	3605(8)	6130(6)	26(1)	1.250
F(2)	3674(7)	4001(8)	8369(6)	26(1)	1.211
F(3)	4215(7)	2282(8)	6014(6)	27(1)	1.043
O(1)	1481(9)	5325(11)	1768(7)	31(2)	2.129
O(2)	1264(10)	6367(11)	3865(8)	31(2)	1.908
O(3)	2908(9)	4225(10)	3686(8)	30(2)	1.687
O(4)	1300(10)	7231(12)	7093(9)	39(2)	1.908
O(5)	2220(9)	9806(12)	7993(9)	38(2)	1.980
O(6)	1944(11)	7552(13)	9378(9)	43(2)	1.958
O(7)	6419(8)	4596(12)	7263(8)	32(2)	1.899
O(8)	8385(9)	5982(11)	8418(8)	29(2)	2.114
O(9)	6155(9)	6758(10)	8772(8)	31(2)	1.904

Table S2. Selected Bond lengths (Å) and angles (deg) for $Rb_3SbF_3(NO_3)_3$.

Sb1—F3	1.957 (4)	Rb3—O7	3.422 (6)
Sb1—F1	1.964 (4)	F1—Rb2^{i}	2.853 (5)
Sb1—F2	1.976 (4)	F2—Rb3^{ix}	2.909 (4)
Sb1—O3	2.528 (5)	O8—N3	1.241 (9)
Sb1—O7	2.567 (6)	O8—Rb1^{x}	2.918 (6)
Rb1—F2	2.850 (5)	O8—Rb1^{ix}	2.920 (6)
Rb1—O8^{ii}	2.918 (6)	O8—Rb2^{xi}	3.110 (6)
Rb1—O8^{iii}	2.920 (6)	O1—N1	1.241 (8)
Rb1—O1^{iv}	2.947 (6)	O1—Rb1^{i}	2.947 (6)
Rb1—O1^{v}	2.983 (5)	O1—Rb3^{xi}	2.959 (6)
Rb1—F1	2.984 (4)	O1—Rb1^{xii}	2.983 (5)
Rb1—O5^{vi}	3.087 (7)	O9—N3	1.252 (9)
Rb1—O6^{vii}	3.154 (7)	O9—Rb3^{xiii}	2.976 (6)
Rb1—O2^{iv}	3.305 (6)	O9—Rb3^{ix}	3.005 (6)
Rb1—O9^{iii}	3.310 (6)	O9—Rb1^{ix}	3.310 (6)
Rb1—O6	3.329 (8)	O2—N1	1.248 (8)
Rb2—O2^{vi}	2.967 (6)	O2—Rb2^{xiii}	2.967 (6)
Rb2—F3	3.001 (5)	O2—Rb2^{i}	3.044 (6)
Rb2—O2^{iv}	3.044 (6)	O2—Rb1^{i}	3.305 (6)
Rb2—O7^{viii}	3.046 (5)	O7—N3	1.263 (9)
Rb2—O4^{iv}	3.057 (6)	O7—Rb2^{xi}	3.046 (5)
Rb2—O5^{vi}	3.058 (6)	O4—N2	1.253 (9)
Rb2—O8^{viii}	3.110 (6)	O4—Rb2^{i}	3.057 (6)
Rb2—O4^{vi}	3.158 (7)	O4—Rb2^{xiii}	3.158 (7)
Rb2—O3	3.459 (6)	N1—O3	1.290 (8)
Rb3—F2^{iii}	2.909 (4)	N1—Rb3^{xi}	3.349 (6)
Rb3—O5^{vi}	2.915 (6)	N1—Rb1^{i}	3.524 (7)
Rb3—F3	2.941 (4)	O5—N2	1.261 (10)

Rb3—O6^{iii}	2.957 (7)	O5—Rb3^{xiii}	2.915 (6)
Rb3—O1^{viii}	2.959 (6)	O5—Rb2^{xiii}	3.058 (6)
Rb3—O9^{vi}	2.976 (6)	O5—Rb1^{xiii}	3.087 (7)
Rb3—O9^{iii}	3.005 (6)	O3—Rb3^{xi}	3.258 (6)
Rb3—O3^{viii}	3.258 (6)	N2—O6	1.232 (9)
F1—Sb1—F2	82.57 (18)	O1^{viii}—Rb3—O9^{iii}	140.52 (16)
F3—Sb1—O3	73.01 (18)	F3—Rb3—O9^{vi}	113.95 (15)
F1—Sb1—O3	78.49 (19)	O6^{iii}—Rb3—O9^{vi}	107.70 (19)
F2—Sb1—O3	153.43 (19)	O1^{viii}—Rb3—O9^{vi}	71.58 (16)
F3—Sb1—O7	71.99 (19)	F2—Rb3—O9^{iii}	65.04 (14)
F1—Sb1—O7	149.67 (19)	F2^{iii}—Rb3—O9^{iii}	60.51 (14)
F2—Sb1—O7	78.01 (18)	O5^{vi}—Rb3—O9^{iii}	71.47 (17)
O3—Sb1—O7	110.40 (18)	F3—Rb3—O9^{iii}	116.57 (15)
O3—Sb1—Rb3	118.34 (12)	O6^{iii}—Rb3—O9^{iii}	83.72 (17)

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

Table S3. Calculation of dipole moment for $Rb(1)O_9F_2$, $Rb(2)O_8F_3$, $Rb(3)O_7F_3$, NO_3 , SbO_3F_3 polyhedra in $Rb_3SbF_3(NO_3)_3$ (D = Debyes).

$Rb_3SbF_3(NO_3)_3$				
Polar unit (a unit cell)	Dipole moment (D)			
	x-component	y-component	z-component	Total magnitude
$Rb(1)O_9F_2$	-2.836320556	-0.821887863	1.383337392	3.260956347
	2.835165953	-0.820001911	-1.38475872	3.260080647
$Rb(2)O_8F_3$	1.795534401	-3.72166525	-0.178400184	4.136008057
	-1.804375064	-3.727718811	0.183548627	4.145521319
$Rb(3)O_7F_3$	-2.679309214	-3.205043346	1.816624821	4.555340432
	2.680770871	-3.205553718	-1.824660649	4.559769028
NO_3	-0.06414	0.020671	0.054841	0.086881
	0.234659	-0.13768	-0.38748	0.473458
	0.377996	-0.13058	-0.00608	0.399962
	-0.35697	-0.13462	0.01462	0.381789
	-0.23329	-0.13635	0.371152	0.459098
	0.064999	0.005515	-0.0372	0.075095
SbO_3F_3	5.854653	15.23312	-4.07241	16.81991
	-5.85447	15.2329	4.072283	16.81962

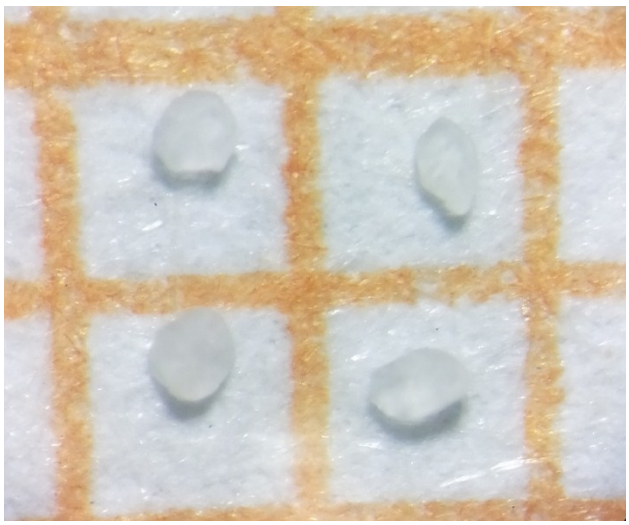

Figure S1. Photograph of $Rb_3SbF_3(NO_3)_3$.

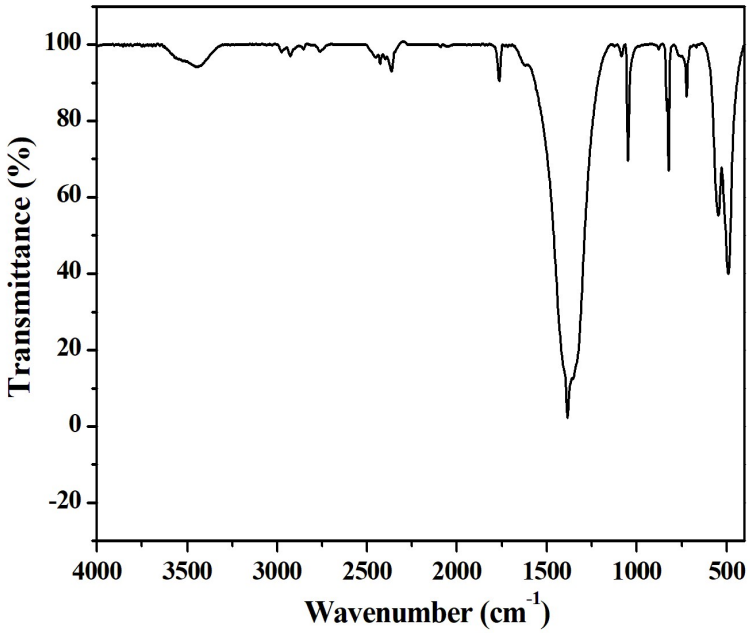

Figure S2. The IR spectrum of $Rb_3SbF_3(NO_3)_3$.

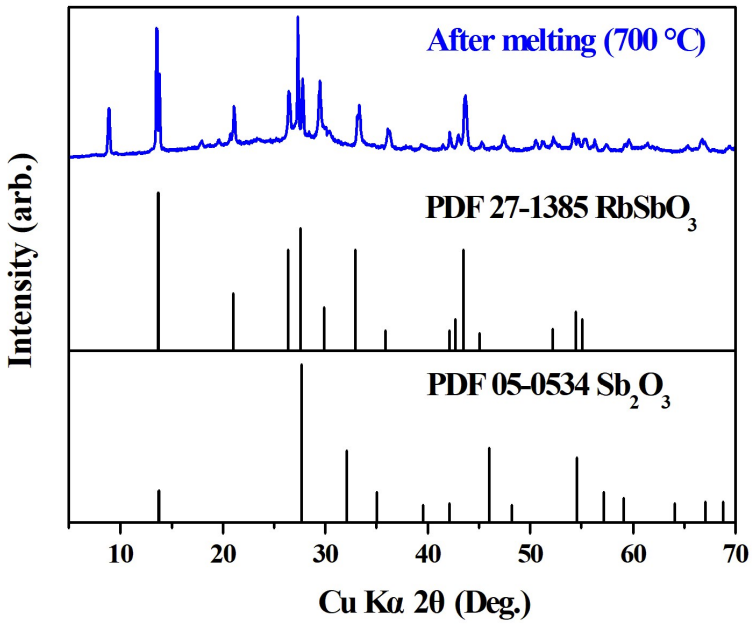

Figure S3. XRD patterns for TGA residues of $Rb_3SbF_3(NO_3)_3$..