Electronic Supporting Information

Low Temperature Molten Salt Synthesis of Noncentrosymmetric $(NH_4)_3SbF_3(NO_3)_3$ and Centrosymmetric $(NH_4)_3SbF_4(NO_3)_2$

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Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $(NH_4)_3SbF_3(NO_3)_3$. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	*x*	*y*	*z*	U_{eq} (Å^2)
Sb1	6394.0 (4)	5429.5 (14)	3668.0 (4)	29.82 (16)
F1	8406 (6)	4325 (7)	3906 (6)	41.0 (11)
F2	5708 (6)	3063 (7)	4045 (6)	44.2 (12)
O1	2264 (11)	5440 (30)	-2068 (10)	87 (2)
O2	3494 (6)	5384 (15)	2765 (6)	46.9 (13)
F3	6262 (6)	4614 (8)	1690 (5)	42.8 (11)
N1	8690 (9)	954 (10)	5274 (9)	41.4 (18)
O3	7072 (8)	5036 (9)	6364 (7)	47.3 (19)
N2	2999 (8)	6547 (11)	1850 (7)	36.8 (15)
O4	8469(10)	6199 (12)	8216 (7)	58 (2)
O5	1621 (8)	6819 (11)	1559 (8)	53.1 (17)
N3	8099 (9)	6132 (10)	6893 (8)	37.2 (15)
O6	2083 (16)	3388 (17)	-606 (14)	96 (3)
O7	3900 (10)	7437 (11)	1284 (8)	49.7 (19)
N4	1919 (9)	3862 (11)	-1839 (8)	39.0 (19)
N5	4555 (10)	1323 (12)	1107 (8)	41.0 (16)

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $(NH_4)_3SbF_4(NO_3)_2$. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	*x*	*y*	*z*	U_{eq} ($Å^2$)
Sb1	6509.2 (2)	7500	5167.3 (2)	21.65 (7)
F1	7535.3 (9)	8611.0 (8)	5779.3 (15)	32.4 (3)
F2	6418.4 (11)	7500	8094 (2)	30.6 (4)
F3	7386.8 (13)	7500	2705 (2)	36.2 (4)
O1	5851.3 (12)	5671.4 (13)	2554 (2)	44.3 (4)
N1	7612.3 (15)	5867.2 (15)	-74 (2)	30.6 (4)
N2	5094.1 (12)	5028.9 (12)	2632 (2)	31.6 (4)
O2	4218.6 (12)	5316.1 (15)	2032 (2)	55.6 (5)
O3	5227.8 (12)	4110.9 (12)	3315 (2)	48.6 (4)
N3	4609 (2)	7500	10275 (4)	37.5 (6)

Table S3. Selected bond distances (Å) and angles (deg) for $(NH_4)_3SbF_3(NO_3)_3$.

Sb1—F1	1.967 (5)	F2—Sb1—F1	85.5 (2)
Sb1—F2	1.921 (5)	F2—Sb1—F3	86.4 (2)
N2—O5	1.240 (10)	F2—Sb1—O3	74.2 (2)
N2—O7	1.250 (11)	F3—Sb1—F1	82.3 (2)
Sb1—F3	1.967 (5)	F3—Sb1—O3	153.5 (2)
Sb1—O3	2.548 (7)	N3—O3—Sb1	110.2 (5)
O1—N4	1.250 (2)	O2—N2—O7	119.6 (8)
O2—N2	1.249 (11)	O5—N2—O2	118.6 (7)
O3—N3	1.265 (10)	O2—N2—O7	121.7 (8)
O4—N3	1.245 (10)	O4—N3—O3	117.7 (8)
N3—O9	1.231 (11)	O9—N3—O3	119.8 (7)
O6—N4	1.212 (15)	O9—N3—O4	122.4 (8)
N4—O8	1.208 (13)	O6—N4—O1	117.2 (10)
F1—Sb1—O3	78.4 (2)	O8—N4—O1	119.2 (10)

Table S4. Selected bond distances (Å) and angles (deg) for $(NH_4)_3SbF_4(NO_3)_2$.

Sb1—F1	1.9407 (10)	F1[1]—Sb1—F2	79.31 (4)
Sb1—F1[1]	1.9407 (10)	F1—Sb1—F2	79.31 (4)
Sb1—F2	2.0731 (14)	F1[1]—Sb1—F3	80.04 (5)
Sb1—F3	2.0672 (14)	F1—Sb1—F3	80.04 (5)
O1—N2	1.247 (2)	F3—Sb1—F2	150.61 (6)
N2—O2	1.240 (2)	O2—N2—O1	119.45 (17)
N2—O3	1.245 (2)	O2—N2—O3	121.03 (17)
F1—Sb1—F1[1]	90.09 (6)	O3—N2—O1	119.52 (16)

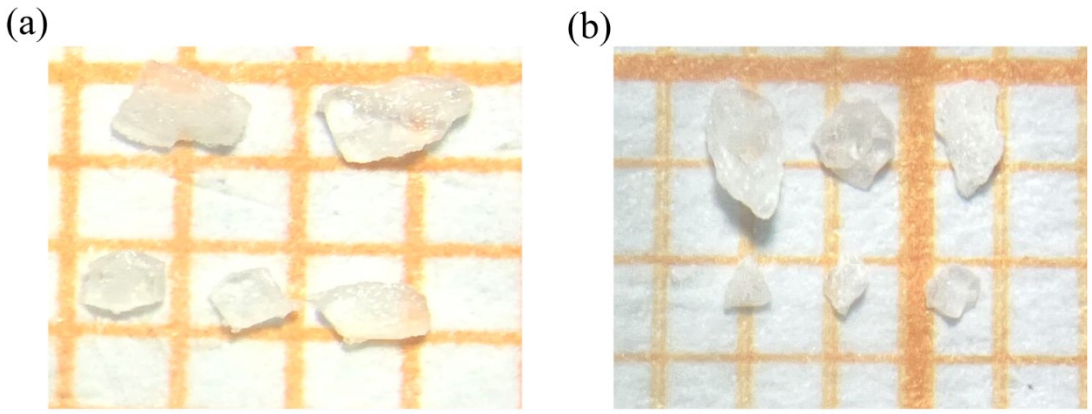

Fig. S1 The crystal photographs of (a) $(NH_4)_3SbF_3(NO_3)_3$ and (b) $(NH_4)_3SbF_4(NO_3)_2$.

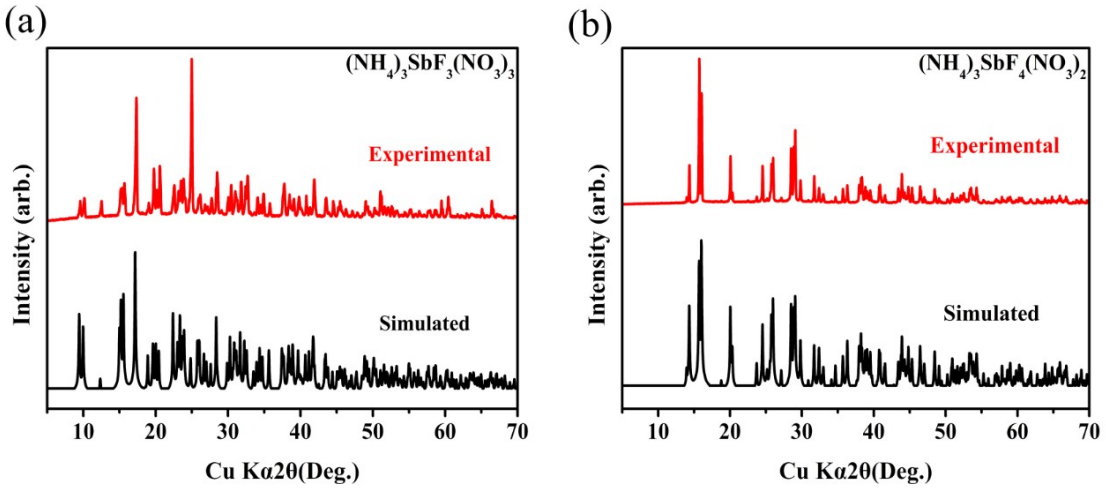

Fig. S2 Experimental and simulated powder XRD patterns for (a) $(NH_4)_3SbF_3(NO_3)_3$ and (b) $(NH_4)_3SbF_4(NO_3)_2$.

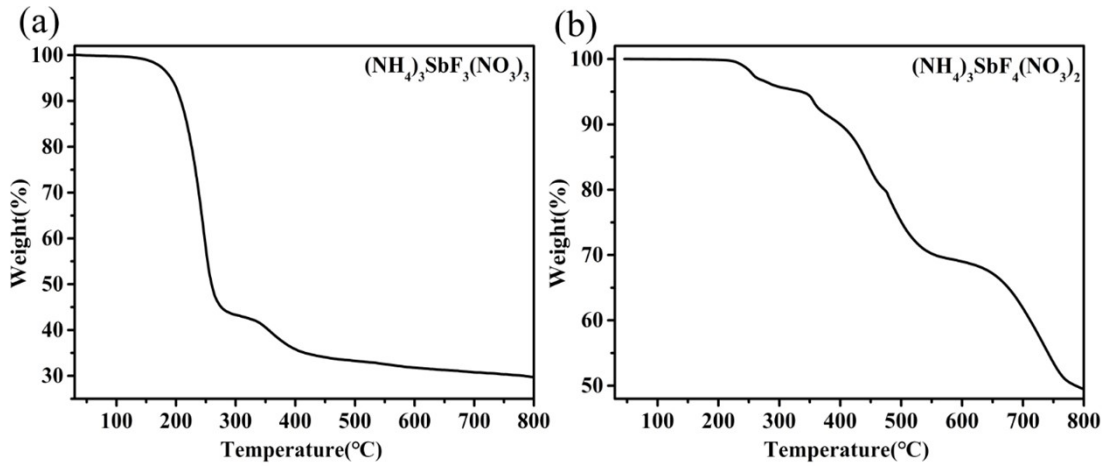

Fig. S3 TGA curves of (a) $(NH_4)_3SbF_3(NO_3)_3$ and (b) $(NH_4)_3SbF_4(NO_3)_2$ under N_2 atmosphere.

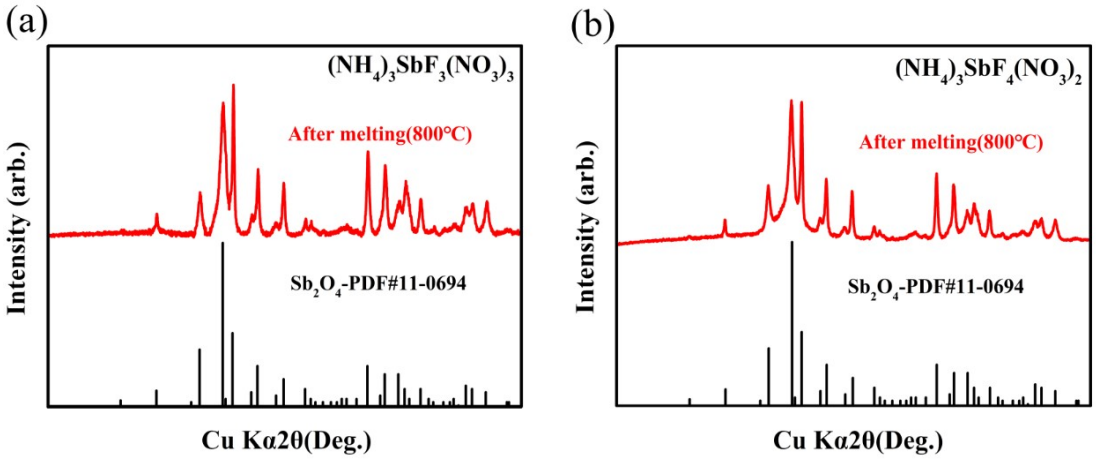

Fig. S4 XRD patterns of (a) $(NH_4)_3SbF_3(NO_3)_3$ and (b) $(NH_4)_3SbF_4(NO_3)_2$ after melting.

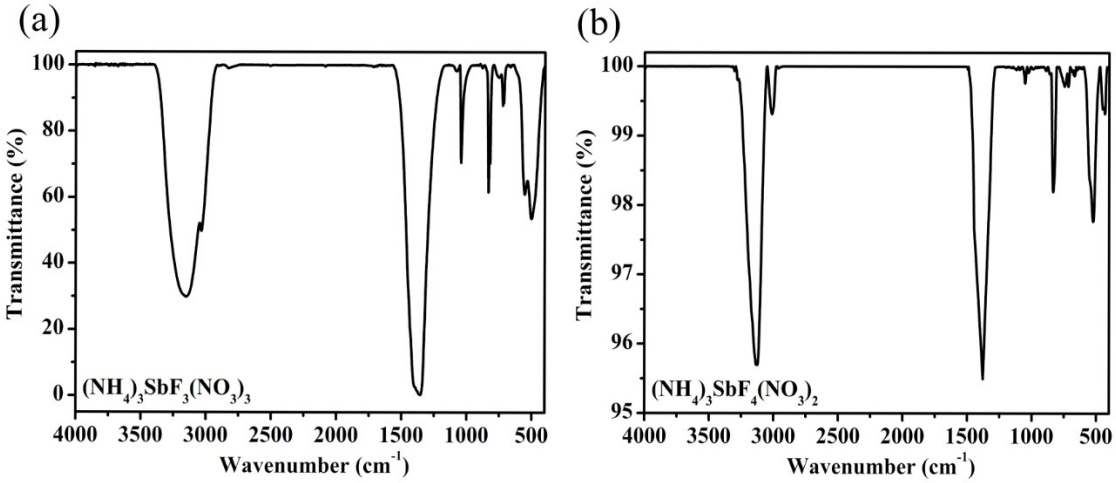

Fig. S5 IR spectra of compounds (a) $(NH_4)_3SbF_3(NO_3)_3$ and (b) $(NH_4)_3SbF_4(NO_3)_2$.

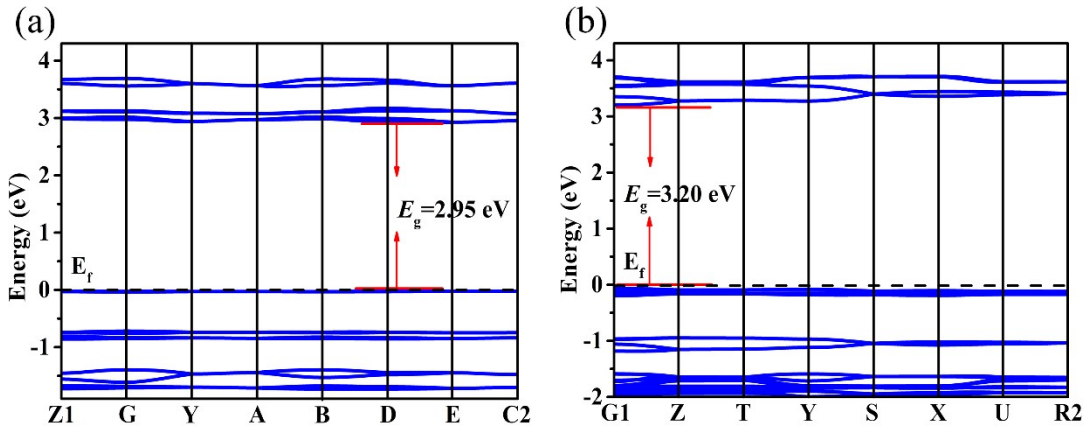

Fig. S6 Calculated band structures for (a) $(NH_4)_3SbF_3(NO_3)_3$ and (b) $(NH_4)_3SbF_4(NO_3)_2$ (the Fermi level is set at 0 eV).