Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting information for

Synergistic Combination of Different Types Functional Motifs in $Rb(NO_3)(SO_3NH_3)$ for Realizing Excellent Ultraviolet Optical Nonlinearity

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Table S1. Crystal Data and Structure Refinement of $Rb(NO_3)(SO_3NH_3)$.

Formula	$H_3N_2O_6RbS$
Formula weight(g/mol)	244.57
Crystal system	Orthorhombic
Space group	*Pmc*2(1)
a/Å	5.6303(3)
b/Å	7.4552(5)
c/Å	8.0537(5)
α/°	90
β/°	90
γ/°	90
Volume/$Å^3$	338.05(4)
Z	2
ρ(calcd) g/cm^3	2.403
μ/mm^{-1}	7.613
F (000)	236
Index ranges	$-7 \le h \le 7$, $-9 \le k \le 9$, $-10 \le l \le 10$
Reflections collected	3669
R_{int}	0.0230
GOF on F^2	1.139
R/wR (I>2 σ(I))	$R_1 = 0.0200$, $wR_2 = 0.0428$
R/wR (all data)	$R_1 = 0.0219$, $wR_2 = 0.0454$
Flack parameter	0.017(15)

[a]$R(F) = \Sigma||F_o| - |F_c||/\Sigma|F_o|\cdot$ wR $(Fo^2) = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^1$

Table S2. Atomic coordinates ($\times 10^4$), equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $Rb(NO_3)(SO_3NH_3)$.

Atom	x	y	z	U(eq)	BVS
Rb	0	3786(1)	5977(1)	35(1)	1.00
S	5000	7137(2)	3770(2)	29(1)	6.19
O(1)	2846(7)	6308(5)	4243(6)	68(1)	-1.77
O(2)	5000	7775(7)	2109(6)	50(1)	-1.73
O(3)	8087(5)	8202(5)	7915(5)	54(1)	-1.66
O(4)	10000	9791(7)	6146(8)	56(1)	-1.73
N(1)	5000	9126(7)	4965(7)	33(1)	-2.93
N(2)	10000	8739(6)	7322(7)	36(1)	5.04

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $Rb(NO_3)(SO_3NH_3)$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Rb	39(1)	35(1)	31(1)	6(1)	0	0
S	29(1)	26(1)	32(1)	0(1)	0	0
O(1)	68(2)	61(3)	75(3)	-16(2)	29(2)	-38(2)
O(2)	78(3)	43(3)	29(3)	0(2)	0	0

O(3)	41(2)	71(3)	51(2)	12(2)	-4(2)	-12(2)
O(4)	76(2)	42(3)	51(3)	20(3)	0	0
N(1)	36(2)	29(3)	32(3)	-3(2)	0	0
N(2)	44(3)	31(3)	32(3)	-3(2)	0	0

Table S4. Bond lengths (Å) and bond angles (°) for $Rb(NO_3)(SO_3NH_3)$.

Rb-O(1)#1	2.837(3)	Rb-N(2)#4	3.495(6)
Rb-O(1)	2.837(3)	Rb-S#7	3.6687(10)
Rb-O(4)#2	2.982(5)	Rb-S#6	3.6687(10)
Rb-O(3)#3	3.072(4)	S-O(1)	1.414(3)
Rb-O(3)#4	3.072(4)	S-O(1)#8	1.414(3)
Rb-O(1)#5	3.081(5)	S-O(2)	1.420(5)
Rb-O(1)#6	3.081(5)	S-N(1)	1.768(5)
Rb-O(2)#6	3.180(2)	O(3)-N(2)	1.244(4)
Rb-O(2)#7	3.180(2)	O(4)-N(2)	1.230(8)
O(1)#1-Rb-O(1)	68.77(19)	O(3)#3-Rb-S#7	132.12(7)
O(1)#1-Rb-O(4)#2	133.17(12)	O(3)#4-Rb-S#7	97.63(7)
O(1)-Rb-O(4)#2	133.17(12)	O(1)#5-Rb-S#7	22.04(7)
O(1)#1-Rb-O(3)#3	74.13(11)	O(1)#6-Rb-S#7	82.60(8)
O(1)-Rb-O(3)#3	97.03(11)	O(2)#6-Rb-S#7	115.78(8)
O(4)#2-Rb-O(3)#3	63.55(14)	O(2)#7-Rb-S#7	22.51(8)
O(1)#1-Rb-O(3)#4	97.04(11)	N(2)#4-Rb-S#7	114.55(5)
O(1)-Rb-O(3)#4	74.13(11)	O(1)#1-Rb-S#6	89.58(10)
O(4)#2-Rb-O(3)#4	63.55(14)	O(1)-Rb-S#6	149.25(9)
O(3)#3-Rb-O(3)#4	41.04(12)	O(4)#2-Rb-S#6	77.57(8)
O(1)#1-Rb-O(1)#5	136.80(9)	O(3)#3-Rb-S#6	97.63(7)
O(1)-Rb-O(1)#5	98.14(13)	O(3)#4-Rb-S#6	132.12(7)
O(4)#2-Rb-O(1)#5	86.47(14)	O(1)#5-Rb-S#6	82.60(8)
O(3)#3-Rb-O(1)#5	148.95(10)	O(1)#6-Rb-S#6	22.04(7)
O(3)#4-Rb-O(1)#5	119.48(9)	O(2)#6-Rb-S#6	22.51(8)
O(1)#1-Rb-O(1)#6	98.14(13)	O(2)#7-Rb-S#6	115.78(8)
O(1)-Rb-O(1)#6	136.81(9)	N(2)#4-Rb-S#6	114.55(5)
O(4)#2-Rb-O(1)#6	86.47(14)	S#7-Rb-S#6	100.23(4)
O(3)#3-Rb-O(1)#6	119.48(9)	O(1)-S-O(1)#8	118.2(4)
O(3)#4-Rb-O(1)#6	148.95(10)	O(1)-S-O(2)	113.6(2)
O(1)#5-Rb-O(1)#6	62.68(15)	O(1)#8-S-O(2)	113.6(2)
O(1)#1-Rb-O(2)#6	83.32(12)	O(1)-S-N(1)	102.7(2)
O(1)-Rb-O(2)#6	152.08(13)	O(1)#8-S-N(1)	102.7(2)
O(4)#2-Rb-O(2)#6	67.74(10)	O(2)-S-N(1)	103.4(3)
O(3)#3-Rb-O(2)#6	75.11(11)	O(1)-S-Rb#9	54.9(2)
O(3)#4-Rb-O(2)#6	111.33(11)	O(1)#8-S-Rb#9	137.87(19)
O(1)#5-Rb-O(2)#6	101.97(11)	O(2)-S-Rb#9	59.02(10)
O(1)#6-Rb-O(2)#6	44.48(10)	N(1)-S-Rb#9	119.41(9)
O(1)#1-Rb-O(2)#7	152.08(13)	O(1)-S-Rb#4	137.86(19)
O(1)-Rb-O(2)#7	83.32(12)	O(1)#8-S-Rb#4	54.9(2)
O(4)#2-Rb-O(2)#7	67.74(10)	O(2)-S-Rb#4	59.02(10)
O(3)#3-Rb-O(2)#7	111.33(11)	N(1)-S-Rb#4	119.41(9)
O(3)#4-Rb-O(2)#7	75.11(11)	Rb#9-S-Rb#4	100.23(4)
O(1)#5-Rb-O(2)#7	44.48(10)	S-O(1)-Rb	155.1(3)

O(1)#6-Rb-O(2)#7	101.97(11)	S-O(1)-Rb#9	103.1(2)
O(2)#6-Rb-O(2)#7	124.58(16)	Rb-O(1)-Rb#9	96.40(10)
O(1)#1-Rb-N(2)#4	86.69(12)	S-O(2)-Rb#9	98.47(14)
O(1)-Rb-N(2)#4	86.69(12)	S-O(2)-Rb#4	98.47(14)
O(4)#2-Rb-N(2)#4	60.01(16)	Rb#9-O(2)-Rb#4	124.58(16)
O(3)#3-Rb-N(2)#4	20.58(6)	N(2)-O(3)-Rb#7	99.2(3)
O(3)#4-Rb-N(2)#4	20.58(6)	N(2)-O(4)-Rb#10	132.2(5)
O(1)#5-Rb-N(2)#4	134.99(9)	O(4)-N(2)-O(3)	120.1(3)
O(1)#6-Rb-N(2)#4	134.99(9)	O(4)-N(2)-O(3)#11	120.1(3)
O(2)#6-Rb-N(2)#4	92.53(10)	O(3)-N(2)-O(3)#11	119.9(5)
O(2)#7-Rb-N(2)#4	92.53(10)	O(4)-N(2)-Rb#7	173.0(4)
O(1)#1-Rb-S#7	149.25(9)	O(3)-N(2)-Rb#7	60.2(3)
O(1)-Rb-S#7	89.58(10)	O(3)#11-N(2)-Rb#7	60.2(3)
O(4)#2-Rb-S#7	77.57(8)		

#1 -x,y,z #2 x-1,y-1,z #3 x-1,-y+1,z-1/2 #4 -x+1,-y+1,z-1/2 #5 x,-y+1,z+1/2 #6 -x,-y+1,z+1/2

#7 -x+1,-y+1,z+1/2 #8 -x+1,y,z #9 -x,-y+1,z-1/2 #10 x+1,y+1,z #11 -x+2,y,z

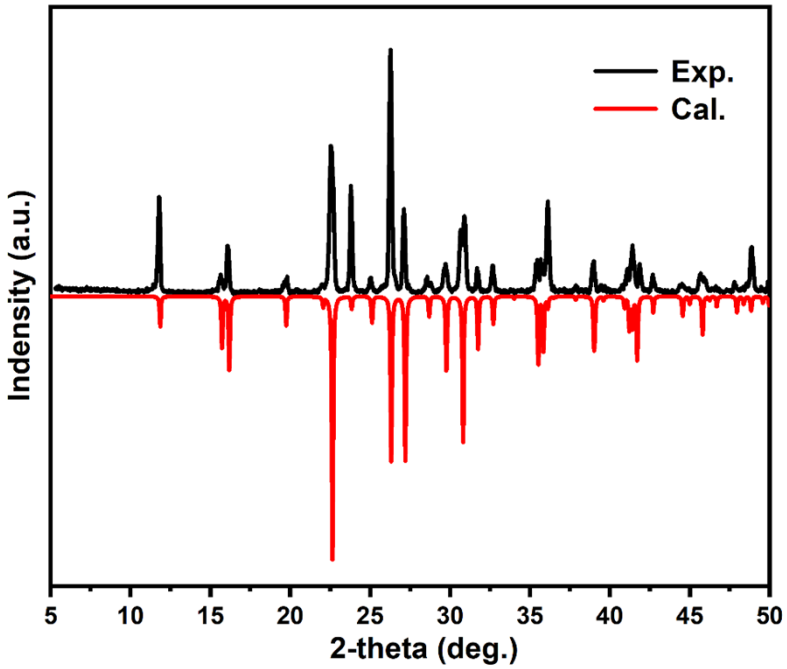

Figure S1. Calculated and experimental powder X-ray diffraction patterns of $Rb(NO_3)(SO_3NH_3)$.

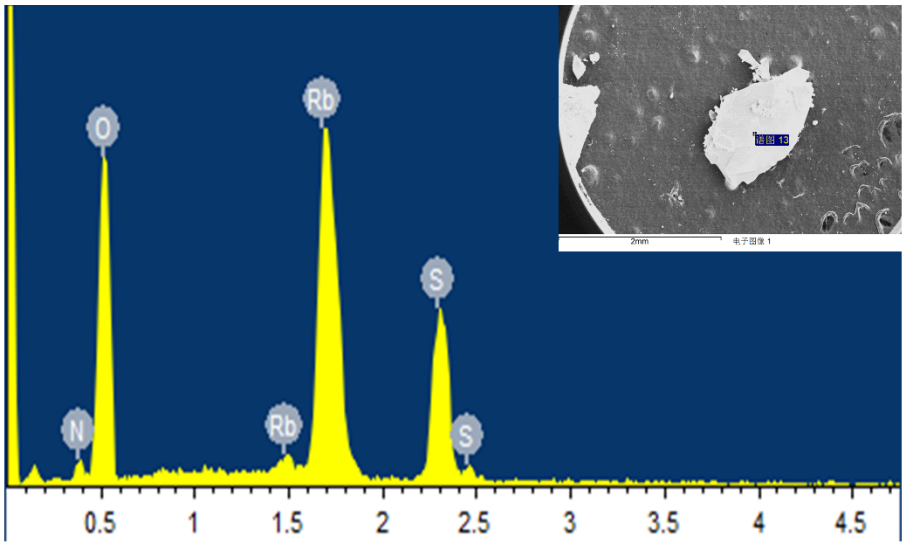

Figure S2. Energy dispersive X-ray spectroscopy analysis of $Rb(NO_3)(SO_3NH_3)$.

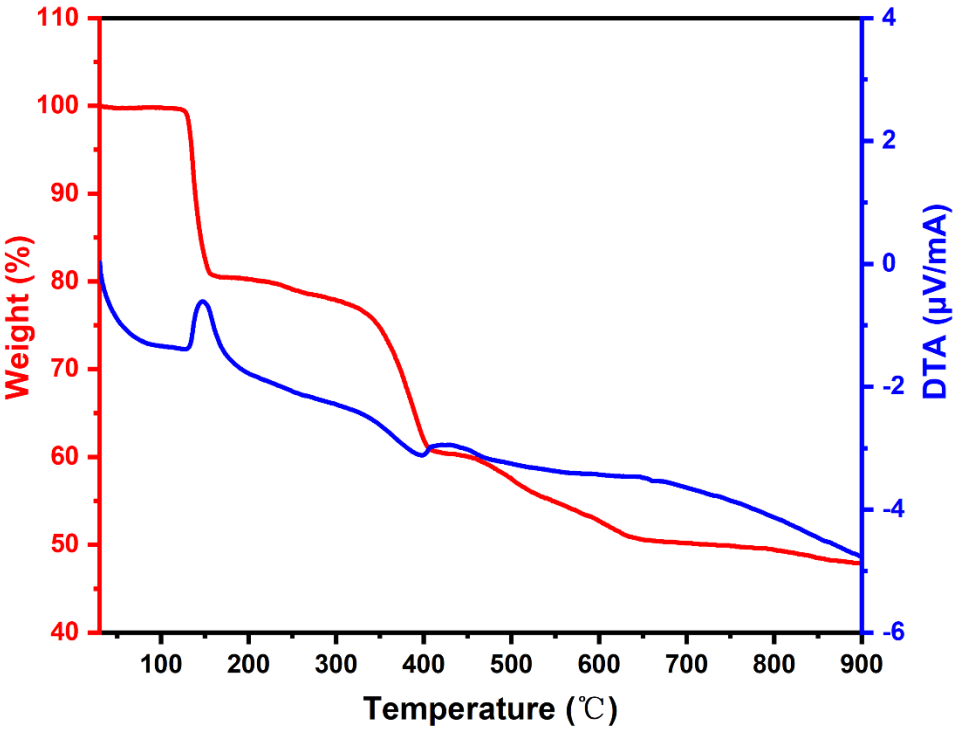

Figure S3. TG-DTA curves of $Rb(NO_3)(SO_3NH_3)$.

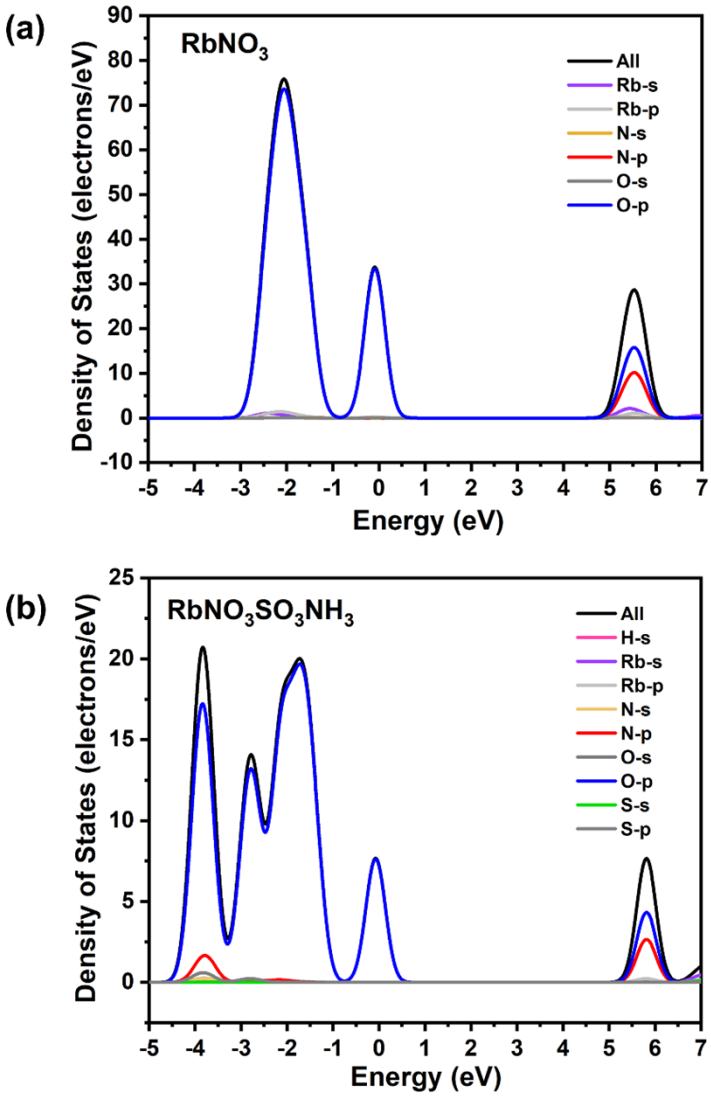

Figure S4. Partial density of states (PDOS) curves for $RbNO_3$ and $Rb(NO_3)(SO_3NH_3)$.

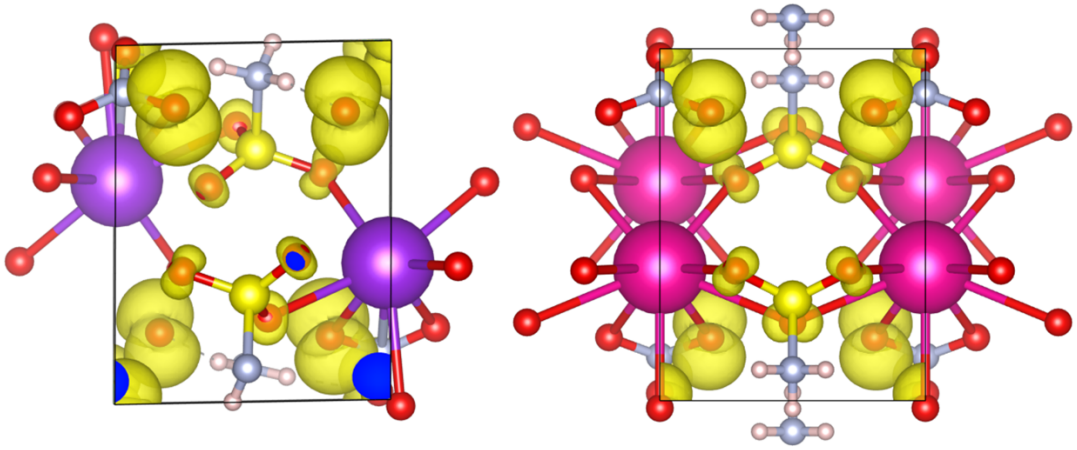

Figure S5. The SHG density of $KNO_3SO_3NH_3$ and $Rb(NO_3)(SO_3NH_3)$.