

Supplementary Materials: $\text{Rb}_2\text{Na}(\text{NO}_3)_3$: A Congruently Melting UV-NLO Crystal with a Very Strong Second-Harmonic Generation Response

Guohong Zou ¹, Chensheng Lin ², Hyung Gu Kim ¹, Hongil Jo ¹ and Kang Min Ok ^{1,*}

Table S1. Selected Bond lengths (Å) and angles (deg) for $\text{Rb}_2\text{Na}(\text{NO}_3)_3$.

Rb1–O1	2.953 (3)	Na1–O6 ^{xiii}	2.696 (6)
Rb1–O1 ⁱ	2.953 (3)	Na1–N2 ^{xii}	2.978 (3)
Rb1–O2 ⁱⁱ	2.958 (5)	Na1–N2 ^{iv}	2.978 (3)
Rb1–O2 ⁱⁱⁱ	2.958 (5)	Na1–Rb1 ^{xiv}	3.928 (2)
Rb1–O4 ^{iv}	2.965 (5)	N1–O2	1.252 (6)
Rb1–O3	3.145 (4)	N1–O2 ^{xiii}	1.252 (6)
Rb1–O3 ^v	3.145 (4)	N1–O1	1.258 (7)
Rb1–O6	3.215 (5)	N1–Rb1 ^{xiv}	3.552 (4)
Rb1–O6 ^v	3.215 (5)	N2–O3 ^v	1.245 (5)
Rb1–O2	3.282 (5)	N2–O3	1.245 (5)
Rb1–O2 ^v	3.282 (5)	N2–O4	1.255 (8)
Rb1–N2	3.363 (6)	N2–Na1 ⁱⁱ	2.978 (3)
Rb2–O4 ^{vi}	2.980 (5)	N2–Na1 ^{xv}	2.978 (3)
Rb2–O2	2.992 (5)	N3–O6 ^{xiii}	1.238 (6)
Rb2–O2 ^v	2.992 (5)	N3–O6	1.238 (6)
Rb2–O5 ^{vii}	3.007 (3)	N3–O5 ^{xvi}	1.244 (8)
Na1–O5	2.337 (6)	O4–Rb2 ^{xvii}	2.980 (5)
Na1–O1	2.337 (6)	O5–N3 ^{xviii}	1.244 (8)
Na1–O3 ^{xi}	2.528 (4)	O5–Rb2 ^{xix}	3.007 (3)
Na1–O3 ^{iv}	2.528 (4)	O5–Rb2 ^{xx}	3.007 (3)
Na1–O4 ^{xii}	2.6585 (12)	O6–Rb2 ^{xix}	3.236 (5)
Na1–O4 ^{iv}	2.6585 (12)	O6–Rb2 ⁱⁱ	3.360 (5)
Na1–O6	2.696 (6)	-	-
O1–Rb1–O1 ⁱ	128.2 (2)	O5–Na1–O4 ^{iv}	89.32 (13)
O1–Rb1–O2 ⁱⁱ	147.25 (15)	O1–Na1–O4 ^{iv}	90.76 (13)
O1 ⁱ –Rb1–O2 ⁱⁱ	84.29 (15)	O3 ^{xi} –Na1–O4 ^{iv}	126.71 (18)
O1–Rb1–O2 ⁱⁱⁱ	84.29 (15)	O3 ^{iv} –Na1–O4 ^{iv}	49.32 (14)
O1 ⁱ –Rb1–O2 ⁱⁱⁱ	147.25 (15)	O4 ^{xii} –Na1–O4 ^{iv}	175.8 (3)
O2 ⁱⁱ –Rb1–O2 ⁱⁱⁱ	63.0 (2)	O5–Na1–O6	89.55 (18)
O1–Rb1–O4 ^{iv}	74.04 (11)	O1–Na1–O6	88.29 (17)
O1 ⁱ –Rb1–O4 ^{iv}	74.04 (11)	O3 ^{xi} –Na1–O6	164.77 (16)
O2 ⁱⁱ –Rb1–O4 ^{iv}	126.29 (12)	O3 ^{iv} –Na1–O6	117.80 (14)
O2 ⁱⁱⁱ –Rb1–O4 ^{iv}	126.29 (12)	O4 ^{xii} –Na1–O6	115.46 (18)
O1–Rb1–O3	111.04 (13)	O4 ^{iv} –Na1–O6	68.48 (16)
O1 ⁱ –Rb1–O3	75.14 (13)	O5–Na1–O6 ^{xiii}	89.55 (18)
O2 ⁱⁱ –Rb1–O3	69.72 (12)	O1–Na1–O6 ^{xiii}	88.29 (17)
O2 ⁱⁱⁱ –Rb1–O3	90.63 (12)	O3 ^{xi} –Na1–O6 ^{xiii}	117.80 (14)
O4 ^{iv} –Rb1–O3	142.94 (12)	O3 ^{iv} –Na1–O6 ^{xiii}	164.77 (16)
O1–Rb1–O3 ^v	75.14 (13)	O4 ^{xii} –Na1–O6 ^{xiii}	68.48 (16)
O1 ⁱ –Rb1–O3 ^v	111.04 (13)	O4 ^{iv} –Na1–O6 ^{xiii}	115.46 (18)
O2 ⁱⁱ –Rb1–O3 ^v	90.63 (12)	O6–Na1–O6 ^{xiii}	47.0 (2)

Table S1. Cont.

O2 ⁱⁱⁱ –Rb1–O3 ^v	69.72 (12)	O5–Na1–N2 ^{xii}	89.68 (14)
O4 ^{iv} –Rb1–O3 ^v	142.94 (11)	O1–Na1–N2 ^{xii}	91.38 (13)
O3–Rb1–O3 ^v	40.01 (15)	O3 ^{xi} –Na1–N2 ^{xii}	24.43 (13)
O1–Rb1–O6	69.34 (14)	O3 ^{iv} –Na1–N2 ^{xii}	101.83 (17)

Symmetry codes: (i) $x - 1, y, z$; (ii) $-x + 1, -y, z - 1/2$; (iii) $x, -y, z - 1/2$; (iv) $-x + 1, -y, z + 1/2$; (v) $-x + 1, y, z$; (vi) $-x + 1, -y - 1, z + 1/2$; (vii) $x, y - 1, z$; (viii) $x - 1, y - 1, z$; (ix) $-x + 1, y - 1, z$; (x) $x, -y, z + 1/2$; (xi) $x + 1, -y, z + 1/2$; (xii) $-x + 2, -y, z + 1/2$; (xiii) $-x + 2, y, z$; (xiv) $x + 1, y, z$; (xv) $-x + 2, -y, z - 1/2$; (xvi) $-x + 2, -y + 1, z - 1/2$; (xvii) $-x + 1, -y - 1, z - 1/2$; (xviii) $-x + 2, -y + 1, z + 1/2$; (xix) $x, y + 1, z$; (xx) $x + 1, y + 1, z$.

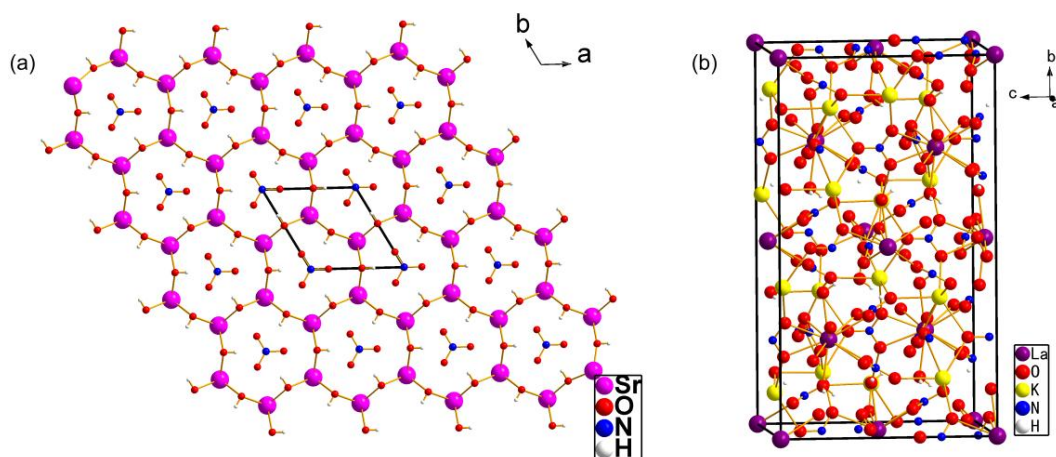


Figure S1. Crystal structure of $\text{Sr}_2(\text{OH})_3\text{NO}_3$ (a) and $\text{K}_2\text{La}(\text{NO}_3)_5 \cdot 2\text{H}_2\text{O}$ (b).

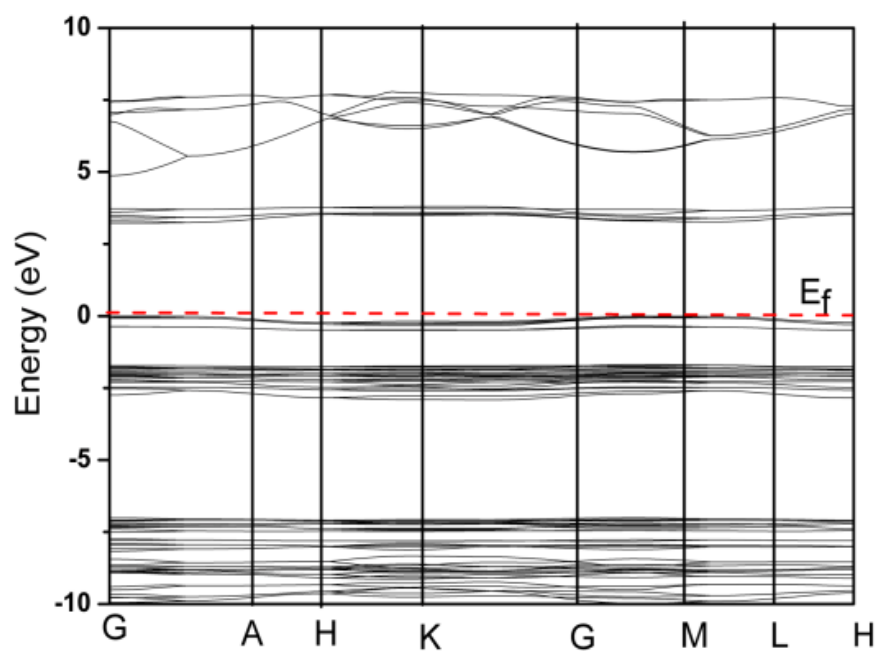


Figure S2. Calculated band structure of $\text{Rb}_2\text{Na}(\text{NO}_3)_3$ (the Fermi level is set at 0 eV).

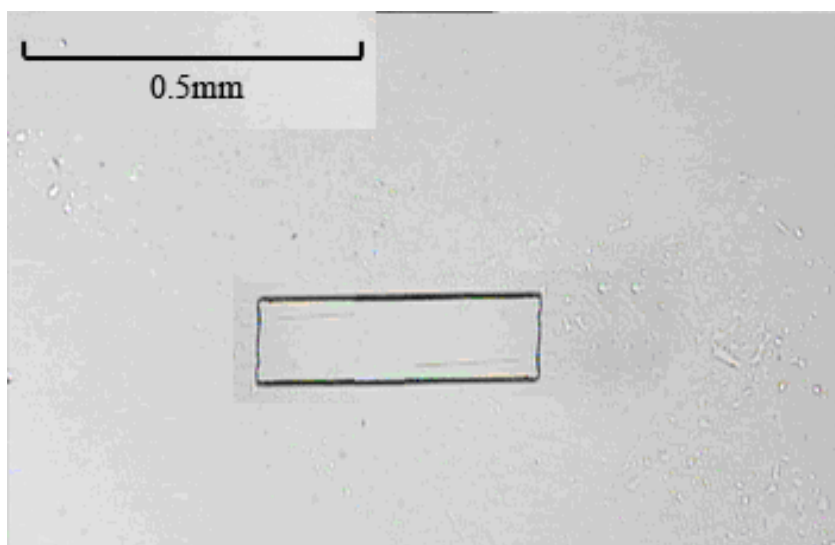


Figure S3. Photograph of Rb₂Na(NO₃)₃ crystal.

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