$Sr_2(OH)_3NO_3$: the First Nitrate as a Deep UV Nonlinear Optical Material with Large SHG Responses

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Table S1. Crystal Data and Structure Refinement for $Sr_2(OH)_3NO_3$.[a]

Formula	$Sr_2(OH)_3NO_3$
Formula Mass (amu)	288.27
Crystal System	Hexagonal
Space Group	*P***Error!**2*m*
a (Å)	6.6037 (2)
c (Å)	3.55850(10)
α(°)	90
γ(°)	120
V(Å^3)	134.392(7)
Z	1
ρ(calcd) (g/cm^3)	3.562
Temperature (K)	293(2)
λ(Å)	1.54184
F(000)	134
μ (mm^{-1})	26.04
Final R indices (I>2σ (I))a R_1/wR_2	0.040/0.104
GOF on F^2	1.24
Absolute Structure Parameter	0.1(2)

[a] $R_1(F) = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2(F_o^2) = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.

Table S2. Selected Bond lengths (Å) and angles (deg) for $Sr_2(OH)_3NO_3$.

Sr1—O2^{i}	2.6259 (13)	Sr1—Sr1^{vii}	3.8127 (1)
Sr1—O2^{ii}	2.6259 (13)	Sr1—H2	2.8421
Sr1—O2^{iii}	2.6259 (13)	O1—N1	1.254 (14)
Sr1—O2^{iv}	2.6259 (13)	O1—Sr1^{viii}	2.798 (10)
Sr1—O2^{v}	2.6259 (13)	N1—O1^{ix}	1.254 (14)
Sr1—O2	2.6259 (13)	N1—O1^{x}	1.254 (14)
Sr1—O1	2.798 (10)	O2—Sr1^{xi}	2.6259 (13)
Sr1—O1^{ii}	2.798 (10)	O2—Sr1^{vi}	2.6259 (13)
Sr1—O1^{iii}	2.798 (10)	O2—Sr1^{xii}	2.6259 (13)
Sr1—Sr1^{v}	3.5585	O2—H2	0.8193
O2^{i}—Sr1—O2^{ii}	136.849 (19)	O2^{iii}—Sr1—Sr1^{vi}	47.35 (3)
O2^{i}—Sr1—O2^{iii}	85.31 (5)	O2^{iv}—Sr1—Sr1^{vi}	132.65 (3)
O2^{ii}—Sr1—O2^{iii}	79.12 (4)	O2^{v}—Sr1—Sr1^{vi}	132.65 (3)
O2^{i}—Sr1—O2^{iv}	79.12 (4)	O2—Sr1—Sr1^{vi}	47.35 (3)
O2^{ii}—Sr1—O2^{iv}	85.31 (5)	O1—Sr1—Sr1^{vi}	90.0
O2^{iii}—Sr1—O2^{iv}	136.849 (19)	O1^{ii}—Sr1—Sr1^{vi}	90.000 (1)
O2^{i}—Sr1—O2^{v}	79.12 (4)	O1^{iii}—Sr1—Sr1^{vi}	90.000 (1)
O2^{ii}—Sr1—O2^{v}	136.849 (19)	Sr1^{v}—Sr1—Sr1^{vi}	180.0
O2^{iii}—Sr1—O2^{v}	136.85 (2)	O2^{i}—Sr1—Sr1^{vii}	43.45 (3)
O2^{iv}—Sr1—O2^{v}	79.12 (4)	O2^{ii}—Sr1—Sr1^{vii}	117.7 (2)
O2^{i}—Sr1—O2	136.85 (2)	O2^{iii}—Sr1—Sr1^{vii}	43.45 (3)
O2^{ii}—Sr1—O2	79.12 (4)	O2^{iv}—Sr1—Sr1^{vii}	117.7 (2)
O2^{v}—Sr1—O2	85.31 (5)	O1—Sr1—Sr1^{vii}	72.9 (2)
O2^{i}—Sr1—O1	71.0 (3)	O1^{ii}—Sr1—Sr1^{vii}	47.1 (2)
O2^{ii}—Sr1—O1	65.9 (3)	O1^{iii}—Sr1—Sr1^{vii}	167.1 (2)
O2^{iii}—Sr1—O1	71.0 (3)	Sr1^{v}—Sr1—Sr1^{vii}	90.0
O2^{iv}—Sr1—O1	65.9 (3)	Sr1^{vi}—Sr1—Sr1^{vii}	90.0
O2^{v}—Sr1—O1	137.21 (5)	O2^{i}—Sr1—H2	120.7
O2—Sr1—O1	137.21 (5)	O2^{ii}—Sr1—H2	91.4

O2^{i}—Sr1—O1^{ii}	65.9 (3)	O2^{iii}—Sr1—H2	70.2
O2^{ii}—Sr1—O1^{ii}	137.21 (5)	O2^{iv}—Sr1—H2	150.7
O2^{iii}—Sr1—O1^{ii}	65.9 (3)	O2^{v}—Sr1—H2	83.7
O2^{iv}—Sr1—O1^{ii}	137.21 (5)	O2—Sr1—H2	16.6
O2^{v}—Sr1—O1^{ii}	71.0 (3)	O1—Sr1—H2	138.0
O2—Sr1—O1^{ii}	71.0 (3)	O1^{ii}—Sr1—H2	54.8
O1—Sr1—O1^{ii}	120.0	O1^{iii}—Sr1—H2	80.4
O2^{i}—Sr1—O1^{iii}	137.21 (5)	Sr1^{v}—Sr1—H2	128.8
O2^{ii}—Sr1—O1^{iii}	71.0 (3)	Sr1^{vi}—Sr1—H2	51.2
O2^{iii}—Sr1—O1^{iii}	137.21 (5)	Sr1^{vii}—Sr1—H2	89.5
O2^{iv}—Sr1—O1^{iii}	71.0 (3)	N1—O1—Sr1	137.1 (2)
O2^{v}—Sr1—O1^{iii}	65.9 (3)	N1—O1—Sr1^{viii}	137.1 (2)
O2—Sr1—O1^{iii}	65.9 (3)	Sr1—O1—Sr1^{viii}	85.9 (4)
O1—Sr1—O1^{iii}	120.0	O1^{ix}—N1—O1	120.000 (1)
O1^{ii}—Sr1—O1^{iii}	120.0	O1^{ix}—N1—O1^{x}	120.0
O2^{i}—Sr1—Sr1^{v}	47.35 (3)	O1—N1—O1^{x}	120.0
O2^{ii}—Sr1—Sr1^{v}	132.65 (3)	Sr1^{xi}—O2—Sr1^{vi}	93.10 (6)
O1—Sr1—Sr1^{v}	90.0	Sr1—O2—Sr1^{xii}	93.10 (6)
O1^{ii}—Sr1—Sr1^{v}	90.000 (1)	Sr1^{xi}—O2—H2	96.7
O2^{i}—Sr1—Sr1^{vi}	132.65 (3)	Sr1—O2—H2	96.8
O2^{ii}—Sr1—Sr1^{vi}	47.35 (3)	Sr1^{xii}—O2—H2	96.7

Symmetry transformations used to generate equivalent atoms:
(i) $-y+1, x-y, z-1$; (ii) $-x+y+1, -x+1, z$; (iii) $-y+1, x-y, z$;
(iv) $-x+y+1, -x+1, z-1$; (v) $x, y, z-1$; (vi) $x, y, z+1$; (vii) $y, x-1, -z$;
(viii) $y+1, x, -z$; (ix) $-y+1, x-y-1, z$; (x) $-x+y+2, -x+1, z$; (xi) $y, x, -z+1$; (xii) $y, x, -z$.

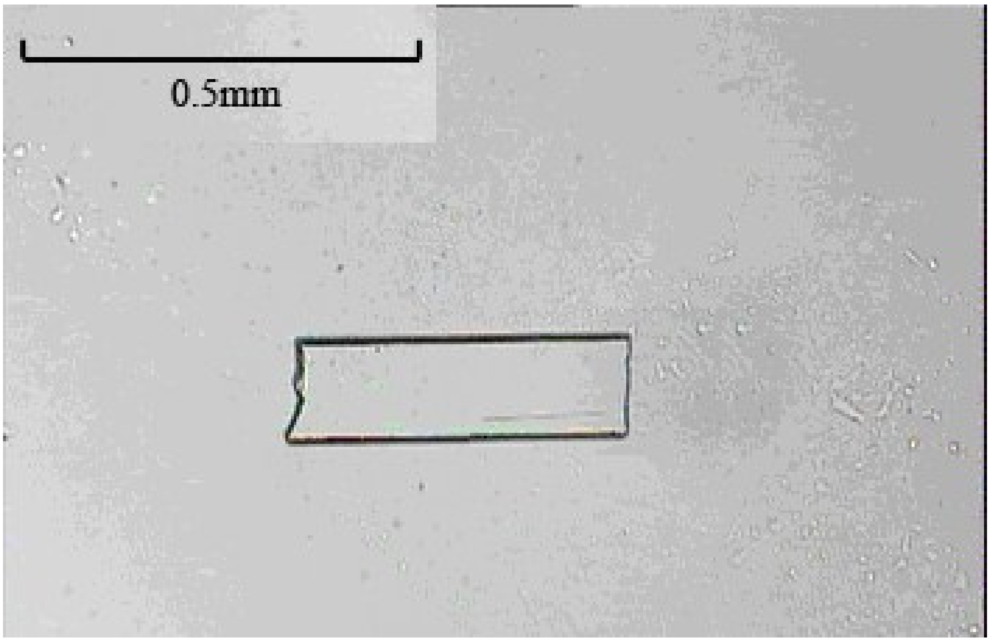

Figure S1. Photograph of $Sr_2(OH)_3NO_3$ crystal.

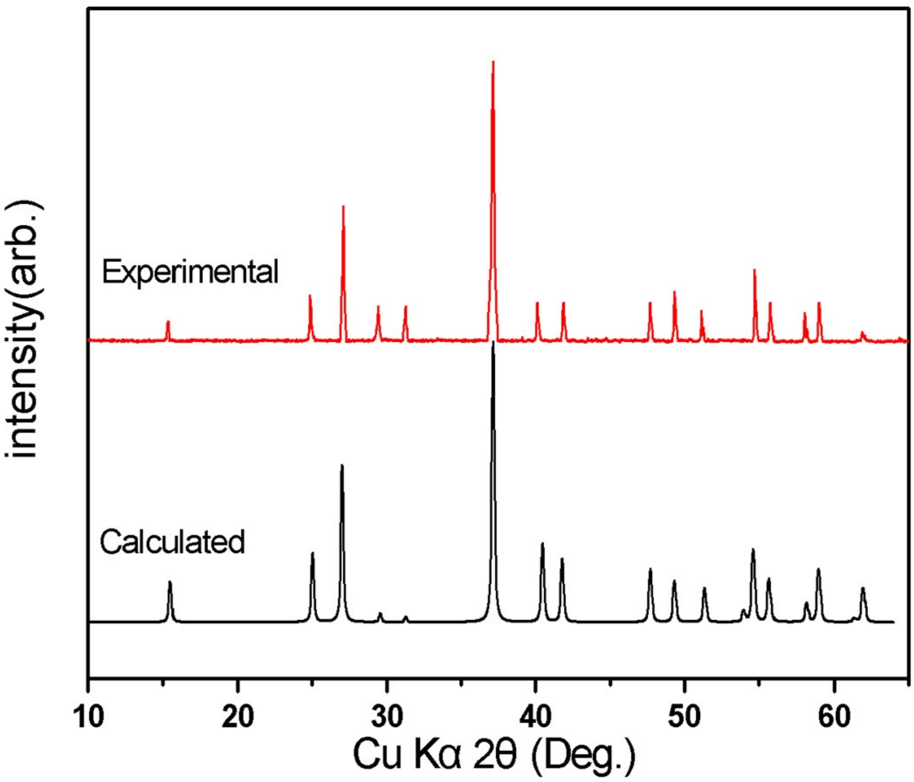

Figure S2. Experimental and calculated XRD patterns for $Sr_2(OH)_3NO_3$. The black curve is the calculated one, the red is the experimental one.

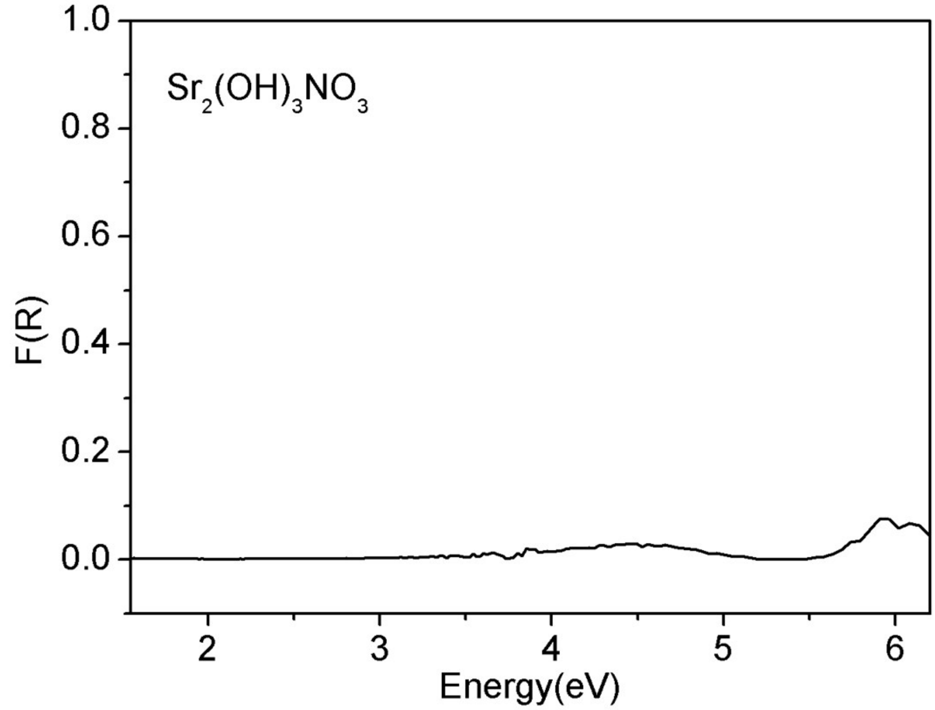

Figure S3. UV absorption spectra and Optical diffuse reflectance spectra of $Sr_2(OH)_3NO_3$.

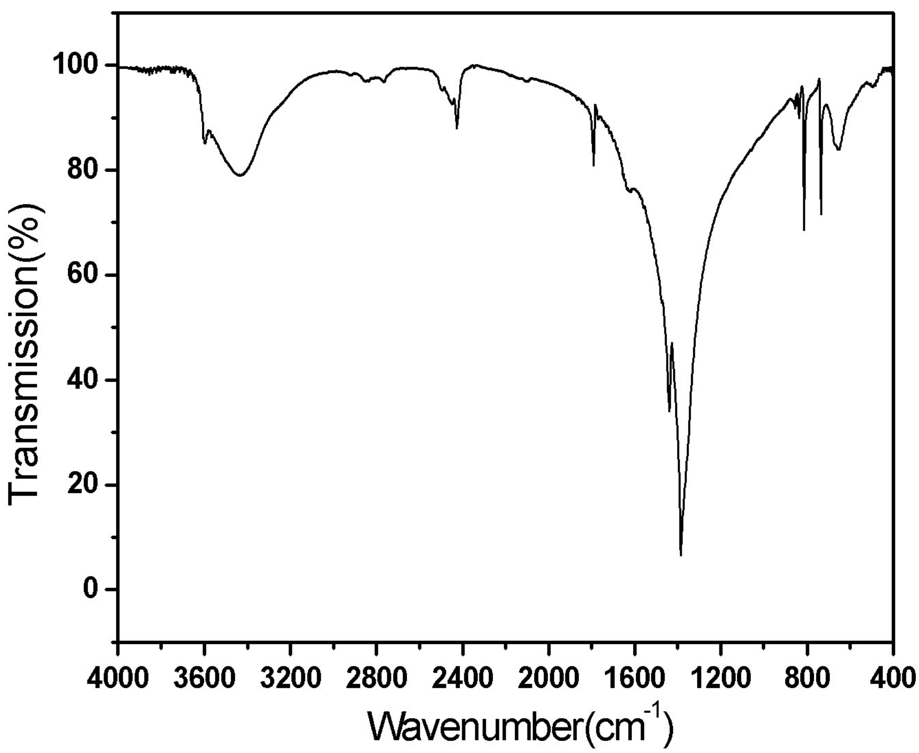

Figure S4. IR spectrum of $Sr_2(OH)_3NO_3$.

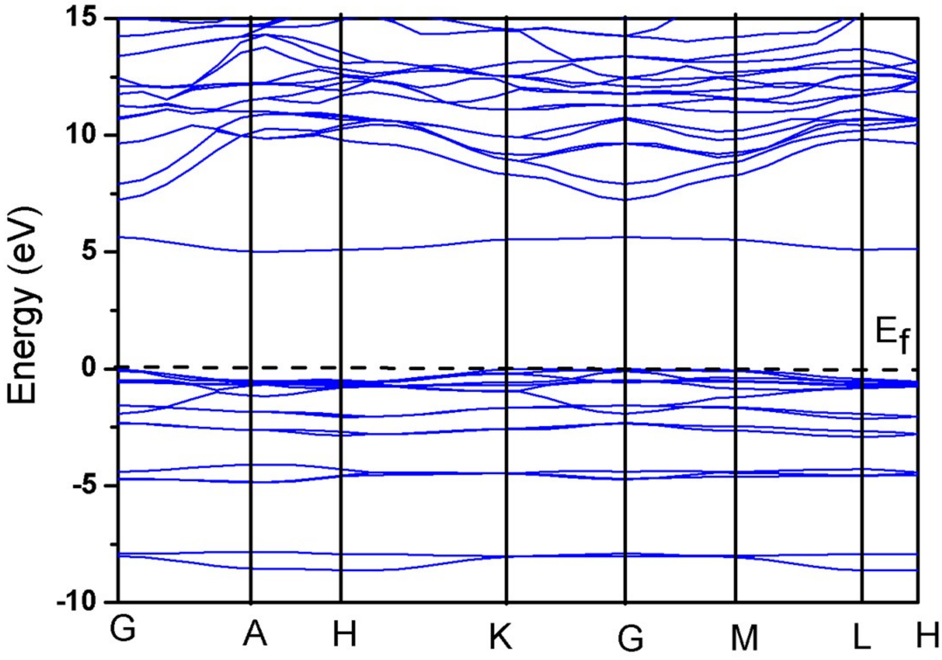

Figure S5. Calculated band structure of $Sr_2(OH)_3NO_3$ (the Fermi level is set at 0 eV).