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The Crystal Structure of Visible Light Absorbing Piezoelectric Semiconductor $SrNb_2V_2O_{11}$ Revisited: High-Resolution X-ray Diffraction, Vibrational Spectroscopy and Computational Study

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Supporting Information

Supplementary data S1.

Full description of HR-PXRD data acquisition at APS 11-BM-B beamline

The 11-BM instrument uses x-ray optics with two platinum-striped mirrors and a double-crystal Si(111) monochromator, where the second crystal has an adjustable sagittal bend. (Wang *et al.*, 2008) Ion chambers monitor incident flux. A vertical Huber 480 goniometer, equipped with a Heidenhain encoder, positions an analyzer system comprised of twelve perfect Si(111) analyzers and twelve Oxford-Danfysik $LaCl_3$ scintillators, with a spacing of 2º 2θ. (Lee *et al.*, 2008) Analyzer orientation can be adjusted individually on two axes. A three-axis translation stage holds the sample mounting and allows it to be spun, typically at ~5400 RPM (90 Hz). A Mitsubishi robotic arm is used to mount and dismount samples on the diffractometer. (Preissner *et al.*, 2009) An Oxford Cryosystems Cryostream Plus device allows sample temperatures to be controlled over the range 80-500 K when the robot is used.

The diffractometer is controlled via EPICS (Dalesio *et al.*, 1994). Data are collected while continually scanning the diffractometer 2θ arm. A mixture of NIST standard reference materials, Si (SRM 640c) and Al_2O_3 (SRM 676) is used to calibrate the instrument, where the Si lattice constant determines the wavelength for each detector. Corrections are applied for detector sensitivity, 2θ offset, small differences in wavelength between detectors, and the source intensity, as noted by the ion chamber before merging the data into a single set of intensities evenly spaced in 2θ.

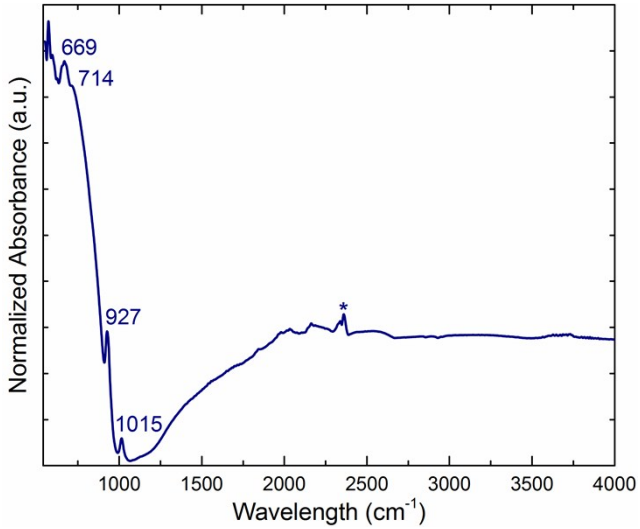

Figure S1. Normalized FTIR absorbance spectrum of $SrNb_2V_2O_{11}$ (* denotes redundant CO_2 vibrational intensity due to background ageing at collection of higher number of scans).

Table S1. Calculated principal components of Born effective charges, their spatial averaged values, relative atomic displacements projections and their cumulative absolute value for model I polytype.

Atom	Z^*_{11}	Z^*_{22}	Z^*_{33}	Z^*_{av}	u_x	u_y	u_z	$\|u\|$
O1	-2.011	-4.172	-1.964	-2.716	-0.0114	0.0001	-0.0158	0.2340
O2	-2.337	-1.220	-6.410	-3.323	-0.0145	0.0048	0.0164	0.3058
O3	-2.301	-5.161	-2.542	-3.335	0.0047	0.0098	0.0191	0.2273
O4	-2.864	-1.005	-0.797	-1.555	-0.0030	0.0239	0.0132	0.2094
O5	-1.971	-4.035	-1.966	-2.657	-0.0024	-0.0069	-0.0083	0.1662
O6	-2.054	-4.102	-1.958	-2.704	-0.0034	-0.0062	-0.0151	0.1713
O7	-2.349	-5.131	-2.501	-3.327	0.0061	0.0012	0.0227	0.2588
O8	-1.914	-0.917	-5.047	-2.626	0.0177	-0.0048	-0.0108	0.3113
O9	-2.080	-0.966	-5.061	-2.703	0.0114	0.0040	-0.0103	0.2251
O10	-2.099	-4.090	-2.009	-2.732	-0.0061	-0.0063	-0.0174	0.1989
O11	-2.844	-0.726	-1.096	-1.555	0.0020	0.0101	0.0303	0.3099
V1	3.628	4.925	4.761	4.438	-0.0021	-0.0003	-0.0062	0.0561
V2	3.639	4.792	4.892	4.441	0.0021	-0.0026	-0.0050	0.0558
Sr1	3.054	2.492	2.561	2.702	-0.0004	-0.0332	-0.0310	0.3624
Nb1	7.263	9.658	9.582	8.834	-0.0016	0.0059	0.0091	0.0724
Nb2	7.240	9.658	9.556	8.818	0.0007	0.0064	0.0091	0.0775

Table S2. Calculated vibrational frequencies for model I (space group Cc)

N vibration	Frequency	Symmetry	IR activity	Raman Activity
1	-0.029173	*A′*	No	No
2	-0.023893	*A″*	No	No
3	-0.017303	*A′*	No	No
4	44.732846	*A″*	Yes	Yes
5	47.934100	*A′*	Yes	Yes
6	59.288383	*A′*	Yes	Yes
7	72.536246	*A″*	Yes	Yes
8	76.529608	*A″*	Yes	Yes
9	78.631310	*A′*	Yes	Yes
10	78.634784	*A″*	Yes	Yes
11	80.725120	*A′*	Yes	Yes
12	83.021207	*A′*	Yes	Yes
13	98.159782	*A″*	Yes	Yes
14	111.357841	*A″*	Yes	Yes
15	119.099900	*A′*	Yes	Yes
16	124.242066	*A″*	Yes	Yes
17	127.875427	*A′*	Yes	Yes
18	128.704661	*A″*	Yes	Yes
19	132.844000	*A″*	Yes	Yes
20	142.469353	*A″*	Yes	Yes
21	144.539000	*A′*	Yes	Yes
22	146.648885	*A″*	Yes	Yes
23	149.007865	*A′*	Yes	Yes
24	151.203529	*A′*	Yes	Yes
25	153.641055	*A′*	Yes	Yes
26	153.901816	*A″*	Yes	Yes
27	165.149439	*A″*	Yes	Yes
28	170.522416	*A′*	Yes	Yes
29	180.673493	*A″*	Yes	Yes
30	182.999556	*A′*	Yes	Yes
31	184.872074	*A″*	Yes	Yes
32	192.014893	*A′*	Yes	Yes
33	195.181271	*A″*	Yes	Yes
34	204.813328	*A″*	Yes	Yes
35	209.062222	*A′*	Yes	Yes
36	215.310731	*A′*	Yes	Yes
37	221.340449	*A″*	Yes	Yes
38	223.799591	*A′*	Yes	Yes
39	240.626824	*A″*	Yes	Yes
40	243.568896	*A′*	Yes	Yes
41	246.434114	*A′*	Yes	Yes
42	248.700776	*A″*	Yes	Yes
43	264.716143	*A″*	Yes	Yes
44	266.930478	*A′*	Yes	Yes
45	268.649539	*A″*	Yes	Yes
46	270.686257	*A′*	Yes	Yes
47	276.809999	*A′*	Yes	Yes
48	282.203761	*A″*	Yes	Yes
49	290.006440	*A′*	Yes	Yes
50	298.444292	*A′*	Yes	Yes
51	302.116840	*A″*	Yes	Yes
52	315.440821	*A″*	Yes	Yes
53	322.450013	*A′*	Yes	Yes
54	331.122925	*A″*	Yes	Yes
55	335.461867	*A″*	Yes	Yes
56	335.986509	*A′*	Yes	Yes
57	337.995705	*A′*	Yes	Yes
58	358.916356	*A′*	Yes	Yes
59	360.021008	*A″*	Yes	Yes
60	365.164812	*A″*	Yes	Yes
61	380.346950	*A″*	Yes	Yes
62	382.026563	*A′*	Yes	Yes
63	385.595445	*A″*	Yes	Yes
64	395.010185	*A″*	Yes	Yes
65	398.652874	*A′*	Yes	Yes
66	401.891026	*A′*	Yes	Yes
67	404.510537	*A′*	Yes	Yes
68	407.613433	*A″*	Yes	Yes
69	412.791258	*A′*	Yes	Yes
70	416.382502	*A″*	Yes	Yes
71	419.346466	*A″*	Yes	Yes
72	419.603664	*A′*	Yes	Yes
73	429.907297	*A″*	Yes	Yes
74	444.223877	*A′*	Yes	Yes

Table S2 (continued)

75	544.108124	*A″*	Yes	Yes
76	545.047920	*A′*	Yes	Yes
77	557.935862	*A′*	Yes	Yes
78	669.011821	*A″*	Yes	Yes
79	693.981157	*A″*	Yes	Yes
80	695.281865	*A′*	Yes	Yes
81	706.278717	*A′*	Yes	Yes
82	706.457727	*A″*	Yes	Yes
83	717.192562	*A′*	Yes	Yes
84	718.764434	*A″*	Yes	Yes
85	719.479573	*A′*	Yes	Yes
86	798.383979	*A′*	Yes	Yes
87	841.680093	*A″*	Yes	Yes
88	858.400592	*A″*	Yes	Yes
89	924.868085	*A′*	Yes	Yes
90	941.523009	*A″*	Yes	Yes
91	944.641949	*A″*	Yes	Yes
92	952.387363	*A′*	Yes	Yes
93	960.355446	*A′*	Yes	Yes
94	976.899430	*A″*	Yes	Yes
95	986.486110	*A″*	Yes	Yes
96	994.300907	*A′*	Yes	Yes

Table S3. Calculated vibrational frequencies for model II (space group Cm)

N vibration	Frequency	Symmetry	IR activity	Raman Activity
1	**-44.625026**	*A″*	Yes	Yes
2	-0.029155*	*A″*	No	No
3	-0.024412*	*A′*	No	No
4	-0.017242*	*A′*	No	No
5	70.560685	*A′*	Yes	Yes
6	74.009740	*A″*	Yes	Yes
7	82.956726	*A′*	Yes	Yes
8	97.150858	*A″*	Yes	Yes
9	124.091524	*A′*	Yes	Yes
10	125.572672	*A″*	Yes	Yes
11	135.571077	*A″*	Yes	Yes
12	149.066976	*A″*	Yes	Yes
13	150.246561	*A′*	Yes	Yes
14	152.734428	*A′*	Yes	Yes
15	160.160540	*A″*	Yes	Yes
16	175.876767	*A″*	Yes	Yes
17	185.978003	*A′*	Yes	Yes
18	191.980447	*A″*	Yes	Yes
19	205.865464	*A′*	Yes	Yes
20	214.183309	*A′*	Yes	Yes
21	243.829827	*A′*	Yes	Yes
22	259.483828	*A″*	Yes	Yes
23	264.363294	*A′*	Yes	Yes
24	300.177443	*A′*	Yes	Yes
25	315.832732	*A″*	Yes	Yes
26	320.726499	*A′*	Yes	Yes
27	339.175697	*A′*	Yes	Yes
28	341.118655	*A″*	Yes	Yes
29	353.277871	*A′*	Yes	Yes
30	371.602602	*A″*	Yes	Yes
31	372.912656	*A′*	Yes	Yes
32	396.776887	*A′*	Yes	Yes
33	403.254116	*A″*	Yes	Yes
34	405.578645	*A′*	Yes	Yes
35	415.042895	*A″*	Yes	Yes
36	423.350364	*A′*	Yes	Yes
37	447.599981	*A′*	Yes	Yes
38	544.550377	*A″*	Yes	Yes
39	547.938107	*A′*	Yes	Yes
40	690.199563	*A′*	Yes	Yes
41	690.942596	*A″*	Yes	Yes
42	718.475138	*A″*	Yes	Yes
43	722.327597	*A′*	Yes	Yes
44	802.000532	*A′*	Yes	Yes
45	927.437740	*A′*	Yes	Yes
46	953.055586	*A′*	Yes	Yes
47	961.556637	*A′*	Yes	Yes
48	1000.920010	*A′*	Yes	Yes

Table S4. Calculated vibrational frequencies for model III (space group C2/c)

N vibration	Frequency	Symmetry	IR activity	Raman Activity
1	**-4.902865**	B_u	Yes	No
2	-0.030786*	B_u	No	No
3	-0.024015*	A_u	No	No
4	-0.018215*	B_u	No	No
5	54.074444	B_g	No	Yes
6	55.883326	A_g	No	Yes
7	56.252109	A_u	Yes	No
8	70.152669	B_g	No	Yes
9	72.846879	B_u	Yes	No
10	73.805926	A_u	Yes	No
11	79.452134	A_g	No	Yes
12	89.181165	A_g	No	Yes
13	95.568144	A_u	Yes	No
14	103.833806	A_u	Yes	No
15	121.735597	B_g	No	Yes
16	127.875918	B_u	Yes	No
17	131.290368	B_g	No	Yes
18	131.291809	A_g	No	Yes
19	138.881920	A_u	Yes	No
20	144.068566	B_u	Yes	No
21	144.498504	B_g	No	Yes
22	148.724668	B_u	Yes	No
23	150.761159	A_g	No	Yes
24	152.373794	A_u	Yes	No
25	154.175956	B_g	No	Yes
26	157.683397	B_u	Yes	No
27	163.982269	A_u	Yes	No
28	170.584782	A_g	No	Yes
29	170.806245	B_u	Yes	No
30	185.105631	A_u	Yes	No
31	189.560269	B_g	No	Yes
32	197.143028	A_u	Yes	No
33	197.152676	A_g	No	Yes
34	198.640841	B_u	Yes	No
35	200.920689	A_g	No	Yes
36	202.675131	B_g	No	Yes
37	212.709606	A_u	Yes	No
38	221.249151	A_g	No	Yes
39	237.360280	B_u	Yes	No
40	239.542828	B_g	No	Yes
41	247.415435	B_u	Yes	No
42	253.767483	B_g	No	Yes
43	255.725671	A_u	Yes	No
44	262.566981	B_g	No	Yes
45	263.343634	A_g	No	Yes
46	265.850644	B_u	Yes	No
47	276.836767	A_g	No	Yes
48	277.821245	A_u	Yes	No
49	281.847391	B_u	Yes	No
50	296.057495	B_g	No	Yes
51	305.414191	A_u	Yes	No
52	311.423019	A_g	No	Yes
53	320.726498	B_u	Yes	No
54	322.168168	A_g	No	Yes
55	330.199980	B_g	No	Yes
56	333.194312	B_g	No	Yes
57	337.443364	A_g	No	Yes
58	346.284425	B_u	Yes	No
59	348.847215	A_u	Yes	No
60	363.505236	A_u	Yes	No
61	370.231778	B_g	No	Yes
62	375.702184	B_u	Yes	No
63	377.289455	A_u	Yes	No
64	393.565366	B_u	Yes	No
65	393.593403	B_g	No	Yes
66	403.434280	B_u	Yes	No
67	407.023555	B_u	Yes	No
68	411.364206	A_u	Yes	No
69	414.043462	A_g	No	Yes
70	415.938040	B_g	No	Yes
71	416.276627	A_g	No	Yes
72	423.745973	B_g	No	Yes
73	424.112899	A_u	Yes	No
74	442.007835	A_g	No	Yes

Table S4 (continued)

75	538.965487	B_u	Yes	No
76	543.065586	A_u	Yes	No
77	558.436825	A_g	No	Yes
78	670.127847	A_u	Yes	No
79	691.461613	B_u	Yes	No
80	698.683582	A_g	No	Yes
81	703.249866	A_u	Yes	No
82	704.928663	B_g	No	Yes
83	709.746278	B_g	No	Yes
84	717.680336	A_u	Yes	No
85	723.443295	A_g	No	Yes
86	800.285059	B_u	Yes	No
87	846.242139	A_u	Yes	No
88	858.320864	B_g	No	Yes
89	926.012525	A_g	No	Yes
90	948.418549	B_g	No	Yes
91	950.833692	A_u	Yes	No
92	956.002749	B_u	Yes	No
93	964.801419	A_g	No	Yes
94	980.038577	A_u	Yes	No
95	984.698180	B_g	No	Yes
96	999.399560	B_u	Yes	No

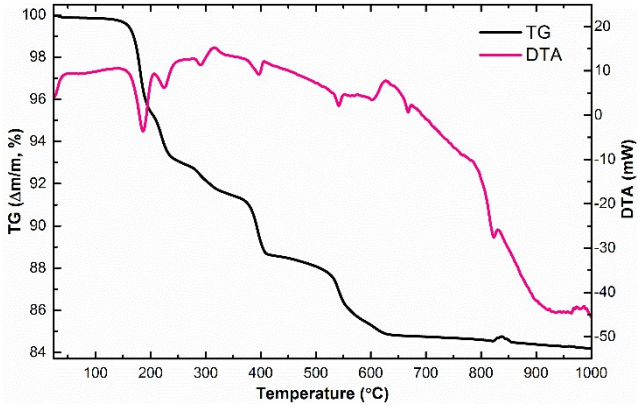

Figure S3. Thermogravimetric (black line) and differential thermal (rose line) analysis traces of stoichiometric reaction mixture.