

Table S1. Powder X-ray data ( $d$  in Å) for nitscheite compared with that calculated from the structure. Only calculated lines with  $I \geq 1.5$  are listed.

$I_{\text{obs}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	$I_{\text{calc}}$	$hkl$
18	8.59	8.6442	12	0 0 2
		6.8614	3	-2 1 1
100	6.45	6.4989	12	-2 0 2
		6.4276	100	0 2 0
		5.7853	8	2 0 2
30	5.69	5.6673	23	-1 0 3
28	5.24	5.2846	18	3 0 1
		5.1579	7	0 2 2
11	4.615	4.5700	10	-2 2 2
		4.3203	6	4 0 0
33	4.275	4.3000	9	2 2 2
		4.2509	24	-1 2 3
38	4.081	4.0828	21	1 2 3
		4.0569	7	-4 0 2
16	3.695	3.6971	12	4 0 2
3	3.583	3.5866	9	0 2 4
22	3.435	3.4672	5	-5 0 1
		3.4314	11	-2 2 4
		3.3162	2	5 0 1
		3.2494	2	-4 0 4
40	3.214	3.2138	15	0 4 0
		3.2048	18	4 2 2
20	3.127	3.1288	17	-3 0 5
11	3.039	3.0525	8	-1 2 5
		3.0122	2	2 4 0
		2.8999	4	-4 2 4
13	2.887	2.8927	2	4 0 4
		2.8814	16	0 0 6
52	2.816	2.8238	12	3 0 5
		2.8132	15	-3 2 5
		2.8094	3	2 4 2
		2.7956	6	-1 4 3

$I_{\text{obs}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	$I_{\text{calc}}$	$hkl$
		2.7461	4	1 4 3
6	2.631	2.6293	14	0 2 6
30	2.591	2.5853	9	3 2 5
		2.5790	2	0 4 4
		2.5194	2	-2 4 4
		2.4255	3	4 4 2
3	2.361	2.3708	2	-7 0 3
8	2.236	2.2418	9	-3 4 5
		2.2243	3	-7 2 3
		2.1663	2	-6 0 6
17	2.151	2.1561	4	-2 0 8
		2.1454	9	0 4 6
		2.1425	3	0 6 0
11	2.122	2.1213	7	3 4 5
		2.0648	3	3 2 7
		2.0528	4	-6 2 6
24	2.048	2.0441	5	-2 2 8
		2.0416	3	2 0 8
		2.0290	2	-4 0 8
		2.0092	2	2 6 2
9	1.9906	2.0040	3	-3 6 1
		1.9856	3	3 6 1
		1.9458	4	2 2 8
12	1.9355	1.9344	4	-8 2 4
		1.9284	2	6 0 6
		1.9082	2	-3 4 7
10	1.8911	1.8947	2	-2 6 4
		1.8853	3	1 0 9
		1.8537	3	4 6 2
12	1.8494	1.8519	3	-1 2 9
		1.8471	4	6 2 6

$I_{\text{obs}}$	$d_{\text{obs}}$	$d_{\text{calc}}$	$I_{\text{calc}}$	$hkl$
13	1.8035	1.8085	4	9 2 1
		1.7963	2	-6 4 6
		1.7905	3	-2 4 8
8	1.7680	1.7769	2	4 2 8
		1.7678	7	-3 6 5
		1.7288	2	0 0 10
8	1.7196	1.7233	3	2 4 8
		1.7193	5	0 6 6
		1.7154	2	-8 4 4
17	1.7039	1.7068	3	3 6 5
		1.7049	5	-5 2 9
4	1.6612	1.6695	2	0 2 10
		1.6536	2	6 4 6
3	1.6272	1.6262	2	1 4 9
4	1.6026	1.6069	2	0 8 0
		1.6021	2	5 0 9
13	1.5516	1.5545	3	5 2 9
		1.5492	3	-5 4 9
6	1.5188	1.5198	2	-2 6 8
		1.5186	2	-3 2 11
2	1.4745	1.4732	4	-4 6 8
		1.4363	2	3 2 11
11	1.4347	1.4333	3	6 6 6
		1.4294	2	-3 8 5
		1.4154	2	1 6 9
11	1.4036	1.4058	2	0 2 12
		1.4051	2	-11 4 3
		1.4034	3	0 8 6
		1.3966	2	3 8 5