

Table S1. Powder X-ray diffraction data (d in Å) for boojumite. Only calculated lines with $I > 1.5$ are listed.

I_{obs}	d_{obs}	d_{calc}	I_{calc}	hkl	I_{obs}	d_{obs}	d_{calc}	I_{calc}	hkl	I_{obs}	d_{obs}	d_{calc}	I_{calc}	hkl
		6.8512	2	0 1 1			2.2892	4	2 8 1			1.7260	2	5 4 3
41	6.52	6.6306	7	2 1 0	7	2.284	2.2837	4	0 3 3			1.7041	3	6 6 2
		6.4507	12	1 0 1			2.2638	5	4 4 2	7	1.6944	1.6984	5	7 3 2
		6.1547	2	1 1 1			2.2189	4	5 0 2			1.6873	4	3 11 1
		4.8980	2	2 3 0	5	2.210	2.2061	2	5 1 2			1.6793	3	5 8 2
10	4.71	4.6965	4	1 3 1			2.2060	2	5 5 1			1.6616	3	0 9 3
		3.8589	2	3 1 1			2.1786	2	0 9 1			1.6592	2	7 4 2
		3.6697	3	3 2 1			2.1712	4	2 7 2			1.6501	2	1 11 2
38	3.559	3.5778	9	0 5 1	7	2.160	2.1527	3	1 9 1	8	1.6540	1.6501	2	1 9 3
		3.5453	14	2 5 0			2.1502	2	3 8 1			1.6486	4	4 7 3
		3.5026	8	4 0 0			2.1386	2	3 1 3			1.6437	4	3 3 4
15	3.411	3.4255	16	0 6 0			2.0977	6	0 8 2			1.6327	2	6 7 2
		3.3276	2	1 2 2	6	2.063	2.0516	2	3 3 3			1.6218	4	2 12 1
5	3.321	3.3153	17	4 2 0			2.0515	6	3 7 2			1.6168	2	2 5 4
		3.1864	17	2 1 2			2.0303	2	6 5 0			1.6158	3	5 6 3
32	3.160	3.1288	10	1 3 2			1.9830	3	4 1 3			1.6158	2	5 10 1
		3.1210	3	3 4 1			1.9644	3	6 0 2	14	1.6130	1.6127	6	4 0 4
		3.1187	3	4 1 1	7	1.9642	1.9583	5	1 10 1			1.6126	2	7 5 2
		3.1186	4	4 3 0			1.9555	4	6 1 2			1.6112	4	8 5 0
		3.0773	3	2 2 2			1.9135	3	3 8 2			1.6081	5	3 4 4
		2.9666	13	0 4 2			1.9033	3	2 10 1			1.5945	2	1 6 4
100	2.911	2.9181	43	2 3 2	13	1.9002	1.9033	2	2 6 3			1.5932	3	4 10 2
		2.9023	14	1 4 2			1.8965	4	7 2 1			1.5730	3	8 5 1
		2.8941	30	4 4 0			1.8883	16	6 3 2			1.5700	2	3 12 1
		2.8677	5	3 0 2			1.8648	2	6 6 1			1.5593	3	8 6 0
		2.8659	4	4 3 1			1.8623	2	5 6 2			1.5449	5	0 13 1
		2.8402	7	3 1 2			1.8574	2	7 3 1			1.5429	4	7 8 1
		2.8401	14	3 5 1	7	1.8535	1.8499	11	4 9 1	11	1.5458	1.5399	2	1 12 2
		2.8337	5	2 6 1			1.8276	5	6 7 0			1.5386	2	4 12 0
		2.7223	2	0 7 1			1.8064	2	7 4 1			1.5356	2	1 7 4
14	2.694	2.7079	12	2 7 0			1.8053	5	2 11 0			1.5202	2	5 1 4
		2.6887	3	4 4 1			1.8016	5	1 0 4			1.5092	2	6 10 1
		2.6724	6	1 5 2			1.7996	12	4 8 2			1.5086	2	2 7 4
		2.6723	2	1 7 1	24	1.7989	1.7947	3	1 1 4	6	1.5056	1.5081	4	8 4 2
		2.6144	3	5 0 1			1.7928	5	4 5 3			1.4919	4	5 8 3
		2.5819	2	3 6 1			1.7890	3	0 2 4			1.4833	2	0 8 4
		2.5691	2	0 8 0			1.7889	6	0 10 2			1.4751	3	1 8 4
5	2.549	2.5337	5	5 2 1			1.7864	2	3 9 2			1.4728	2	8 5 2
		2.5217	3	4 0 2			1.7745	2	1 10 2	8	1.4643	1.4614	4	5 4 4
		2.4490	2	4 2 2			1.7726	2	4 10 0			1.4591	5	4 6 4
		2.4056	2	0 1 3			1.7702	3	5 7 2			1.4589	2	6 11 0
		2.3665	2	4 3 2			1.7513	5	8 0 0					
		2.3519	2	3 5 2			1.7486	8	1 8 3					
10	2.331	2.3250	8	1 2 3	10	1.7471	1.7467	3	7 5 1					
		2.3201	6	6 1 0			1.7424	3	1 3 4					