Supplementary Table S1. Calculated powder diffraction pattern of vapnikite (Cu$K\alpha_{1+2}$ = 1.540598, geometry: Debye-Scherrer, no anomalous dispersion; condition: $I > 2.00$)

h	k	l	d_{hkl}	I_{rel}	h	k	l	d_{hkl}	I_{rel}	h	k	l	d_{hkl}	I_{rel}
0	1	1	4.8384	78	–3	0	1	1.8672	3	–1	4	1	1.4193	2
–1	0	1	4.7389	28	3	0	1	1.8610	2	1	4	1	1.4184	3
1	0	1	4.7058	39	–1	1	4	1.8603	10	–1	2	5	1.4091	3
0	0	2	4.1558	36	–2	2	2	1.8535	13	2	3	3	1.4033	3
1	1	0	4.1306	79	1	1	4	1.8522	12	–2	1	5	1.4024	4
0	2	0	2.9753	47	2	2	2	1.8455	10	0	4	2	1.4006	6
–1	1	2	2.9376	100	–1	3	1	1.8297	2	–3	2	3	1.3952	2
1	1	2	2.9218	99	3	1	0	1.8210	8	–1	3	4	1.3936	5
2	0	0	2.8692	43	–1	3	2	1.7104	19	1	3	4	1.3902	5
–1	2	1	2.5198	17	1	3	2	1.7073	18	3	2	3	1.3876	2
1	2	1	2.5148	8	0	2	4	1.7036	23	–4	1	1	1.3771	3
0	1	3	2.5116	11	–2	0	4	1.6890	10	3	3	0	1.3769	3
1	0	3	2.4877	14	2	0	4	1.6770	12	–3	1	4	1.3744	3
–2	1	1	2.4727	21	–3	1	2	1.6723	24	3	1	4	1.3647	3
2	1	1	2.4632	6	3	1	2	1.6636	22	–4	0	2	1.3592	2
0	2	2	2.4192	11	0	3	3	1.6128	3	2	4	0	1.3207	6
–2	0	2	2.3695	5	–2	3	1	1.6023	4	–1	1	6	1.3155	8
2	0	2	2.3529	5	0	1	5	1.6010	5	1	1	6	1.3112	8
1	1	3	2.2952	2	2	3	1	1.5997	4	–3	3	2	1.3091	6
0	0	4	2.0779	24	1	0	5	1.5935	2	3	3	2	1.3049	7
2	2	0	2.0653	47	–3	2	1	1.5815	3	4	2	0	1.2922	7
0	3	1	1.9293	6	–3	0	3	1.5796	3	–2	4	2	1.2599	4
–1	2	3	1.9151	9	3	2	1	1.5778	4	2	4	2	1.2574	4
1	2	3	1.9085	4	0	4	0	1.4876	5	0	2	6	1.2558	3
–2	1	3	1.8963	4	–2	2	4	1.4688	11	4	1	3	1.2421	2
2	1	3	1.8835	7	2	2	4	1.4609	11	–4	2	2	1.2363	3
1	3	0	1.8747	15	4	0	0	1.4346	5	4	2	2	1.2316	3
										0	4	4	1.2096	4