

Appendix

Table S1. Simulated X-ray powder diffraction data for jianmuite ($I \geq 1.0$, d in Å)

I	d (Å)	h	k	l	I	d (Å)	h	k	l
13.7	7.127	0	1	1	32.2	1.685	2	4	4
13.8	7.127	1	0	1	32.2	1.685	2	4	-4
9.4	4.192	2	1	1	1.3	1.672	5	3	2
9.2	4.192	2	1	-1	1.3	1.672	5	3	-2
1.3	4.077	1	1	2	27.5	1.639	6	2	0
1.3	4.077	1	1	-2	1.4	1.621	2	3	5
6.1	3.665	2	2	0	1.4	1.621	2	3	-5
1.9	3.563	0	2	2	2.5	1.598	4	5	-1
2.0	3.563	2	0	2	2.6	1.598	4	5	1
1.6	2.759	3	2	-1	1.1	1.565	1	5	-4
1.5	2.759	3	2	1	1.1	1.565	1	5	4
1.1	2.726	1	3	-2	1.3	1.547	1	4	5
1.1	2.726	1	3	2	1.4	1.547	1	4	-5
100.0	2.726	3	1	-2					
99.6	2.726	3	1	2	1.3	1.527	6	3	-1
2.2	2.673	2	1	-3	1.3	1.527	6	3	1
2.0	2.673	2	1	3	1.8	1.464	0	7	1
1.5	2.592	4	0	0	1.7	1.464	7	0	1
8.6	2.453	0	0	4	8.9	1.463	3	1	-6
2.7	2.436	1	4	-1	9.0	1.463	3	1	6
2.8	2.436	1	4	1	1.5	1.451	4	5	-3
3.3	2.376	0	3	3	1.5	1.451	4	5	3
3.2	2.376	3	0	3	1.0	1.438	4	6	0
1.2	2.326	1	1	-4	7.8	1.405	5	5	2
1.3	2.326	1	1	4	7.5	1.405	1	7	-2
16.8	2.318	2	4	0	7.5	1.405	1	7	2
6.0	2.160	3	2	-3	7.7	1.405	5	5	-2
6.0	2.160	3	2	3	1.3	1.383	0	4	6
6.0	2.096	4	2	2	1.3	1.383	4	0	6
6.0	2.096	4	2	-2	3.6	1.363	6	2	-4
5.4	1.993	1	4	3	3.6	1.363	6	2	4
1.5	1.993	4	1	-3					
5.3	1.993	1	4	-3	1.2	1.342	2	1	7
1.5	1.993	4	1	3	1.1	1.342	2	1	-7
1.8	1.928	1	0	5	3.1	1.227	0	0	8
1.8	1.928	0	1	5	1.0	1.218	2	8	-2
4.6	1.889	5	2	1	1.1	1.210	1	1	-8
4.8	1.889	5	2	-1	1.1	1.210	1	1	8
1.2	1.878	1	5	2	1.5	1.204	3	8	1
1.2	1.878	1	5	-2	1.6	1.204	3	8	-1
1.7	1.728	6	0	0	4.4	1.159	4	8	0

Note: Two lines at the same 2θ are treated as one in identifying the 7 strongest lines. The intensity is halved when only one of the two lines is intense enough to be listed.