

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

I_{obs}	d_{obs}	d_{calc}	I_{calc}	hkl
100	10.38	10.3648	100	0 1 0
37	8.89	8.8981	39	1 0 0
13	8.15	8.2753	5	0 1 1
		8.0406	10	1 0 1
38	7.24	7.2402	36	1 1 1
		7.0206	3	1 1 0
17	5.922	5.9257	15	-1 0 1
		5.7283	3	1-1 1
8	5.132	5.1824	2	0 2 0
		5.0979	2	0 2 1
		5.0909	6	0 1 2
6	5.003	4.9884	4	-1-1 1
3	4.331	4.3370	2	-1 2 0
3	4.247	4.2766	3	0-2 1
4	4.095	4.0900	4	2 1 2
6	3.985	3.9836	5	-1 0 2
4	3.890	3.8962	4	-1 1 2
		3.7963	3	2 2 1
6	3.726	3.7084	2	1 1 3
		3.7043	5	-2 0 1
9	3.630	3.6201	10	2 2 2
5	3.473	3.4725	4	-2-1 1
3	3.270	3.2664	3	1-2 2
7	3.154	3.1574	4	1-1 3
		3.1410	2	-1 3 0
8	3.093	3.0852	5	-1 3 1
		3.0821	3	0-3 1
8	2.965	2.9628	7	-2 0 2
4	2.885	2.8933	2	-1-3 1
		2.8828	2	2-1 3

I_{obs}	d_{obs}	d_{calc}	I_{calc}	hkl
7	2.859	2.8653	4	3-1 1
		2.8497	5	3 2 2
		2.7420	2	2 3 3
8	2.700	2.6954	7	1 2 4
7	2.643	2.6530	5	0 4 1
		2.6334	2	-2 3 0
		2.5912	2	0 4 0
8	2.551	2.5455	6	0 2 4
		2.5403	2	1 4 0
5	2.516	2.5100	5	3-2 1
6	2.459	2.4534	5	-1-3 2
3	2.325	2.3177	2	-1 4 2
2	2.211	2.2067	2	4-1 1
11	2.177	2.1749	10	4-1 2
9	2.118	2.1091	8	-2-4 1
13	2.083	2.0837	4	0 2 5
		2.0772	3	1 3 5
		2.0753	3	2 3 5
6	2.053	2.0509	4	-1-4 2
7	1.9863	1.9900	3	-4 2 0
		1.9740	2	0 3 5
6	1.8042	1.7980	5	-2-5 1
11	1.7851	1.7854	2	5-1 2
		1.7841	4	5-1 1
		1.7792	5	1 3 6
3	1.7271	1.7239	2	5 2 0
5	1.6437	1.6335	2	5 3 0
5	1.5242	1.5185	2	5 1 6
5	1.4966	1.4988	3	-3 4 4
5	1.4674	1.4624	3	2 7 4