Table S1. Calculated X-ray powder diffraction data ($I_{calc} > 1$) for hollisterite (in Å for Cu$K\alpha$1, Bragg-Brentano geometry), calculated using the the cell parameters and the atomic coordinates (space group $C2/m$) given by Freiburg and Grushko (1994) with site occupancies modified from the empirical formula from this study, using Powder Cell version 2.4. The strongest reflections are given in bold.

h	*k*	*l*	*d* (Å)	I_{calc}
2	0	0	7.4140	3
-2	0	1	7.4091	4
1	1	0	6.9997	6
-1	1	1	6.4606	15
1	1	1	5.6790	33
2	0	1	5.5630	4
-2	0	2	5.5568	2
-1	1	2	4.8999	5
1	1	2	4.2353	6
3	1	0	4.1961	1
2	0	2	4.0630	28
-2	0	3	4.0589	26
0	2	0	3.9700	19
0	0	3	3.9637	29
-3	1	2	3.9547	1
-4	0	1	3.9000	2
0	2	1	3.7657	1
4	0	0	3.7070	21
-4	0	2	3.7045	14
3	1	1	3.6652	3
2	2	0	3.4998	43
-2	2	1	3.4993	12
-3	1	3	3.3571	3
0	2	2	3.3016	17
4	0	1	3.2627	4
-4	0	3	3.2593	6
2	2	1	3.2315	12
-2	2	2	3.2303	15
2	0	3	3.1161	8
0	0	4	2.9727	5
2	2	2	2.8395	1
-4	0	4	2.7784	3
5	1	0	2.7782	6
4	2	0	2.7095	3
-5	1	3	2.6692	3
1	3	0	2.6055	1
-6	0	1	2.5849	2
5	1	1	2.5461	1
4	2	1	2.5207	4
-4	2	3	2.5191	8
2	0	4	2.5036	1
2	2	3	2.4512	7
-1	3	2	2.4358	1
0	2	4	2.3796	5
-3	3	1	2.3558	3
-3	1	5	2.3522	2
1	3	2	2.3399	5
3	3	0	2.3332	11
-3	3	2	2.2891	21
-6	0	4	2.2803	1
4	2	2	2.2780	2
-4	2	4	2.2763	3
5	1	2	2.2757	5
-1	3	3	2.2339	20
3	3	1	2.2286	3
-6	2	1	2.1662	2
-6	2	2	2.1658	1
1	1	5	2.1575	22
-3	3	3	2.1535	22
-7	1	2	2.1434	1
-5	1	5	2.1404	17
-7	1	1	2.1266	2
1	3	3	2.1246	9
2	2	4	2.1177	2
6	**2**	**0**	**2.0980**	**100**
-6	**2**	**3**	**2.0970**	**85**
-7	1	3	2.0926	7
2	0	5	2.0841	41
-2	0	6	2.0828	39
3	3	2	2.0711	17
6	0	2	2.0659	24
-6	0	5	2.0636	44
7	1	0	2.0467	25
0	**2**	**5**	**2.0401**	**79**
4	**2**	**3**	**2.0321**	**84**
-4	**2**	**5**	**2.0305**	**82**
5	1	3	2.0159	6
-3	1	6	2.0082	8
-5	3	2	2.0020	8
0	**4**	**0**	**1.9850**	**83**
-1	1	6	1.9847	8
0	0	6	1.9818	3
5	3	0	1.9746	24
-8	0	2	1.9500	29
-5	3	3	1.9344	11
-8	0	1	1.9246	1
-8	0	3	1.9240	2

Table S2. Calculated X-ray powder diffraction data ($I_{calc} > 1$) for kryachkoite (in Å for Cu$K\alpha$1, Bragg-Brentano geometry), calculated using the the cell parameters, atomic coordinates (space group $Cmc2_1$) given by Black et al. (1961) with site occupancies modified from the empirical formula from this study, using Powder Cell version 2.4. The strongest reflections are given in bold.

h	*k*	*l*	*d* [Å]	I_{rel}
1	**1**	**0**	**4.8722**	**38**
0	0	2	4.3885	19
1	1	1	4.2599	11
2	0	0	3.7300	14
1	1	2	3.2608	25
0	2	0	3.2170	12
0	2	1	3.0205	4
2	0	2	2.8421	11
0	2	2	2.5946	15
1	1	3	2.5082	23
2	2	0	2.4361	10
2	2	1	2.3474	5
3	1	0	2.3195	2
3	**1**	**1**	**2.2425**	**61**
0	0	4	2.1943	25
0	**2**	**3**	**2.1644**	**35**
2	**2**	**2**	**2.1299**	**87**
1	**3**	**0**	**2.0612**	**46**
3	**1**	**2**	**2.0507**	**100**
1	**3**	**1**	**2.0066**	**32**
1	**1**	**4**	**2.0007**	**62**
2	0	4	1.8913	8
2	2	3	1.8721	16
1	3	2	1.8657	2
4	0	0	1.8650	8
3	1	3	1.8176	4
0	2	4	1.8127	8
4	0	2	1.7164	5
1	3	3	1.6850	2
1	1	5	1.6515	1
2	2	4	1.6304	8
4	2	0	1.6135	2
0	4	0	1.6085	3
3	3	1	1.5970	1
3	1	4	1.5940	5
0	2	5	1.5409	4
3	3	2	1.5231	6
4	2	2	1.5144	13
0	4	2	1.5103	1
1	3	4	1.5023	4
2	4	0	1.4770	5
0	0	6	1.4628	4
2	4	1	1.4565	14
5	1	0	1.4534	2
2	2	5	1.4242	1
3	3	3	1.4200	2
4	2	3	1.4129	10
0	4	3	1.4095	1
2	4	2	1.3999	5
3	1	5	1.3997	6
2	0	6	1.3619	7
1	3	5	1.3364	4
0	2	6	1.3316	3
2	4	3	1.3185	6
3	3	4	1.3054	9
5	1	3	1.3017	7
4	2	4	1.2999	2
0	4	4	1.2973	17
1	5	0	1.2681	1
1	5	1	1.2550	1
2	2	6	1.2541	13
6	0	0	1.2433	12
3	1	6	1.2373	9
2	4	4	1.2253	1
5	3	0	1.2248	12
1	5	2	1.2182	1
4	4	0	1.2181	1
1	1	7	1.2143	1
5	3	1	1.2130	9
5	1	4	1.2117	13
4	4	1	1.2065	4

Table S3. Calculated X-ray powder diffraction data ($I_{calc} > 1$) for stolperite (in Å for Cu$K\alpha$1, Bragg-Brentano geometry), calculated using the the cell parameters, atomic coordinates (space group Pm-3m) given by Zhang et al. (2005) with site occupancies modified from the empirical formula from this study, using Powder Cell version 2.4. The strongest reflections are given in bold.

h	*k*	*l*	*d* (Å)	I_{rel}
1	**0**	**0**	**2.9000**	**20**
1	**1**	**0**	**2.0506**	**100**
1	1	1	1.6743	6
2	**0**	**0**	**1.4500**	**17**
2	1	0	1.2969	7
2	**1**	**1**	**1.1839**	**34**
2	2	0	1.0253	10
3	0	0	0.9667	1
2	2	1	0.9667	2
3	**1**	**0**	**0.9171**	**12**
3	1	1	0.8744	1
2	2	2	0.8372	3
3	2	0	0.8043	1
3	**2**	**1**	**0.7751**	**12**
4	0	0	0.7250	1
4	1	0	0.7034	1
3	2	2	0.7034	1
4	1	1	0.6835	3
3	3	0	0.6835	2
3	3	1	0.6653	0
4	2	0	0.6485	3
4	2	1	0.6328	1
3	3	2	0.6183	2
4	2	2	0.5920	2
5	0	0	0.5800	0
4	3	0	0.5800	0
5	1	0	0.5687	1
4	3	1	0.5687	3