

Supplementary material P-XRD

Table S1a. The powder X-ray diffraction pattern of zinconigerite-2N1S

<i>I</i> _{obs.}	<i>d</i> _{obs.}	<i>d</i> _{cal.}	<i>h</i>	<i>k</i>	<i>l</i>
5	4.666	4.658	1	0	1
8	4.030	4.023	1	0	2
74	2.841	2.833	1	0	4
100	2.431	2.428	1	1	3
17	2.181	2.180	2	0	3
16	2.012	2.012	2	0	4
5	1.986	1.987	1	1	5
25	1.851	1.853	2	1	1
34	1.834	1.835	1	0	7
2	1.807	1.806	2	1	2
4	1.731	1.728	0	0	8
74*	1.646	1.645	2	1	4
12	1.632	1.632	1	0	8
81	1.545	1.549	2	1	5
4	1.478	1.479	1	1	8
32	1.428	1.428	2	2	0
27	1.417	1.416	3	0	5
28*	1.365	1.364	2	2	3
1	1.347	1.347	3	1	2
3	1.331	1.331	1	0	10
21	1.275	1.275	3	1	4
9	1.230	1.232	4	0	1
7	1.217	1.218	1	0	11
3	1.163	1.165	4	0	4
4	1.149	1.151	1	1	11
7	1.130	1.130	4	0	5
1	1.120	1.120	2	0	11
15	1.079	1.080	4	1	0
39*	1.050	1.050	3	2	5
11	1.043	1.043	2	1	11
9	1.006	1.006	4	0	8

*: Peaks overlapping with fluorite peaks.

Table S1b. The powder X-ray diffraction pattern of zinconigerite-6N6S

<i>I</i> _{obs.}	<i>d</i> _{obs.}	<i>d</i> _{cal.}	<i>h</i>	<i>k</i>	<i>l</i>
2	4.199	4.195	1	0	7
34	2.846	2.849 {	1	0	16
			1	1	0
5	2.722	2.717	0	1	17
6	2.584	2.592	1	1	9
17	2.525	2.519	1	0	19
15	2.489	2.492	0	2	1
100	2.436	2.436	0	2	4
39	2.424	2.417	0	1	20
6	2.099	2.101	2	0	14
2	2.014	2.012	0	2	16
16	1.971	1.971	2	0	17
100*	1.931	1.936	1	1	21
17	1.892	1.891	0	2	19
5	1.870	1.869	1	2	2
5	1.859	1.855	2	1	4
4	1.844	1.849	0	0	30
3	1.811	1.806	1	2	8
3	1.783	1.781	0	1	29
1	1.770	1.769	0	2	22
9	1.679	1.677	0	0	33
100*	1.650	1.650	3	0	0
100*	1.646	1.645	2	1	16
12	1.636	1.630	0	1	32
18	1.625	1.626	1	2	17
4	1.575	1.576	2	1	19
62	1.553	1.554	0	3	12
15	1.549	1.549 {	1	2	20
			1	0	34
5	1.515	1.514	2	0	29
15	1.499	1.501	2	1	22
14	1.442	1.448	0	2	31
61	1.430	1.429	2	2	0
18	1.421	1.419	2	0	32
5	1.400	1.400	2	2	8
9	1.348	1.347	3	1	8
6	1.331	1.333	1	3	10
7	1.235	1.235	0	4	3
21*	1.222	1.223	4	0	7
2	1.201	1.208	0	4	10
8	1.130	1.130	3	2	5
18	1.085	1.081	4	1	0
9	1.078	1.078	4	1	4
5	1.000	0.991	0	5	0
11	0.988	0.988	0	5	4
27	0.955	0.953	4	1	27
7	0.946	0.946	3	3	7
41	0.935	0.936	2	4	1
17	0.933	0.933	4	2	2
40*	0.911	0.913	4	2	14
2	0.894	0.899	4	0	43
5	0.889	0.889	5	1	1
10	0.879	0.878	1	5	10

Data were obtained using a DMAX RAPID II micro-diffractometer (MoK α). Unit cell parameters were refined using the method of Holland and Redfern (1997). *: Peaks overlapping with fluorite peaks.