

Table S1. Calculated X-ray powder diffraction data for machiite ($I_{\text{rel}} > 1$).

<i>h</i>	<i>k</i>	<i>l</i>	<i>d</i> [Å]	<i>I</i> _{rel}					
2	0	0	8.176	100	-2	0	4	1.758	2
1	1	0	4.808	4	-4	0	4	1.751	5
4	0	0	4.088	51	-9	1	2	1.728	1
3	1	0	3.697	24	9	1	0	1.709	30
-2	0	2	3.502	2	4	2	2	1.695	35
0	0	2	3.376	41	-10	0	2	1.677	15
-4	0	2	3.083	2	-6	0	4	1.670	12
-1	1	2	2.882	79	-3	1	4	1.665	1
2	0	2	2.841	5	-1	1	4	1.637	30
-3	1	2	2.783	15	10	0	0	1.635	3
5	1	0	2.742	79	-5	1	4	1.626	2
6	0	0	2.725	3	3	3	0	1.603	2
1	1	2	2.657	18	-8	2	2	1.580	3
0	2	0	2.515	30	8	0	2	1.558	1
-6	0	2	2.509	7	1	1	4	1.551	4
-5	1	2	2.441	45	-8	0	4	1.541	1
2	2	0	2.404	10	-1	3	2	1.513	12
4	0	2	2.294	12	6	2	2	1.501	5
3	1	2	2.278	1	-3	3	2	1.498	2
2	2	1	2.205	7	5	3	0	1.492	15
-7	1	1	2.195	6	1	3	2	1.478	3
4	2	0	2.142	13	-2	2	4	1.441	2
7	1	0	2.119	7	-5	3	2	1.437	24
-3	1	3	2.118	6	-4	2	4	1.437	4
-7	1	2	2.057	4	3	1	4	1.432	8
-2	2	2	2.043	1	11	1	0	1.426	3
-8	0	2	2.031	3	4	0	4	1.421	3
0	2	2	2.017	18	-12	0	2	1.415	1
-4	2	2	1.949	1	-9	1	4	1.410	3
5	1	2	1.911	1	0	2	4	1.402	1
2	2	2	1.883	3	-10	0	4	1.396	7
6	0	2	1.870	5	-10	2	2	1.395	14
6	2	0	1.848	3	-6	2	4	1.391	12
-6	2	2	1.776	6	9	1	2	1.379	12