

Table 2. X-ray powder diffraction data (d in Å, I in %) for vanpeltite

h	k	l	I_{cal}	I_{meas}	d_{cal}	d_{meas}
0	0	2	19.3	9.8	11.577	11.578
1	0	-1	100.0	100.0	8.058	8.072
1	0	-3	64.7	76.4	5.749	5.751
1	1	0	3.8	5.4	4.494	4.507
1	1	2	12.1	14.4	4.197	4.199
1	1	4	68.2	91.2	3.549	3.555
0	1	5	36.0	60.0	3.471	3.485
2	1	1	43.2	58.4	3.301	3.304
2	1	3	7.0	11.1	3.069	3.062
2	0	6	4.3	7.8	2.871	2.870
0	1	7	10.3	11.6	2.808	2.805
-2	1	5	2.0	2.6	2.707	2.710
0	2	0	13.9	16.0	2.641	2.646
3	1	0	3.5	3.2	2.520	2.522
1	1	-8	5.3	11.4	2.442	2.437
2	0	8	6.5	13.1	2.399	2.399
-3	1	4	1.8	3.7	2.316	2.313
3	0	-7	5.5	6.9	2.172	2.169
-3	1	6	2.5	6.9	2.111	2.113
2	1	-9	3.6	4.7	2.043	2.039
1	2	-7	1.9	1.8	2.013	2.010
-4	1	3	8.0	18.0	1.938	1.931
3	2	5	6.7	11.4	1.798	1.792
2	2	8	7.3	18.3	1.781	1.777
0	2	10	1.1	2.4	1.740	1.742
3	1	10	2.3	4.1	1.705	1.704
-3	2	7	1.9	2.1	1.678	1.677
1	3	4	4.8	11.1	1.653	1.655
2	3	1	3.6	3.8	1.628	1.628
4	2	4	1.5	0.9	1.599	1.603
4	1	9	2.9	6.9	1.574	1.574
0	2	12	2.4	4.3	1.559	1.559
3	1	-12	1.2	2.5	1.532	1.534
3	3	0	0.8	1.5	1.504	1.502
1	3	-8	1.1	1.8	1.485	1.484
1	2	-13	1.4	1.5	1.455	1.457
5	2	1	2.4	1.6	1.440	1.440
3	2	-11	1.1	0.6	1.427	1.429
2	1	-15	0.5	1.2	1.402	1.402
-6	1	1	0.6	2.9	1.380	1.382
-4	3	3	1.6	2.2	1.344	1.343
0	4	0	1.6	2.6	1.322	1.323

-1	4	1	0.7	0.9	1.307	1.305
1	4	-3	1.1	2.9	1.289	1.289
3	3	10	0.6	2.8	1.259	1.260
-2	4	4	1.0	2.1	1.235	1.235
2	2	-16	0.6	0.9	1.219	1.218
2	3	13	0.7	2.6	1.203	1.203

Refined unitcell parameters are: $a=8.6058(4)$, $b=5.2912(1)$, $c=23.1553(9)$,
 $\beta=90.110(3)$, $V=1054.38(4)$.