Short Communication

Cell Dimensions of Boltwoodite. By TOSHIO KATO and YASUNORI MIÚRA, *Department of Mineralogical Sciences and Geology, Faculty of Literature and Science, Yamaguchi University, Yoshida, Yamaguchi 753*

ABSTRACT

Cell dimensions of boltwoodite, $K(H_3O)(UO_2)(SiO_4) \cdot O \cdot 1H_2O$, have been determined using electron and X-ray powder diffraction data: a 13.71(1), b 7.14(1), c 12.35(2) Å, β 102.1(1)°, V 1187(3) Å³. $Z=6$. $G_{meas.}=3.6$, $G_{calc.}=3.52(OH_2O)-3.68(1H_2O)$. The newly indexed X-ray powder data for sklodowskite and kasolite are given.

Boltwoodite, $K(H_3O)(UO_2)(SiO_4) \cdot O \cdot 1H_2O$, is an alkali uranyl silicate mineral first described and named by Frondel and Ito (1956) who studied a specimen from the Delta mine, Emery County, Utah. Physical, chemical, differential thermal and X-ray diffraction data and the results of hydrothermal synthesis were recorded by Honea (1961) but its powder diffraction data could not be indexed due to the small size of available crystals.

Fine dispersions of boltwoodite from the type locality supplied by British Museum (BM 1961, 283) and Dr. K. Sakurai have now been examined by electron microscopy and single-crystal electron diffraction patterns for the preferred orientation on (100) taken by the crystals on the stage of the microscope operated at an accelerating voltage of 150 kV.

The specimens were heavily shadowed by aluminum to give reference diffraction rings for calibration purposes. The electron diffraction pattern showed a rectangular array of intensities and gave the following trial value for cell parameters, *viz.*, $b=7.08$, $c=11.99$ Å, $\alpha=90^\circ$. X-ray powder diffraction data by Honea were referred

Table 1. X-ray powder data for boltwoodite.

<i>hkl</i>	<i>d</i> (calc.) Å	<i>I</i>	<i>d</i> (obs.*) Å	<i>hkl</i>	<i>d</i> (calc.) Å	<i>I</i>	<i>d</i> (obs.*) Å
		2	7.53	236	1.455	1	1.455
200	6.733	10	6.81	806	1.438	1	1.438
201	6.441	5	6.40	145	1.412	3	1.411
201	5.452	5	5.45	028	1.394	1	1.393
211	4.783	4	4.74	920, 428	1.380	2	1.378
211	4.333	4	4.32	715	1.356	1B	1.356
202	4.121	2	4.11	10.1.3	1.335	2	1.335
212	4.103			352	1.311	2	1.311
301	3.965	1	3.91	832	1.297	4B	1.297
310	3.800	1	3.75	10.2.3	1.270	0.5	1.270
113	3.550	7	3.54	833	1.242	2B	1.242
401	3.420	9	3.40	545, 11.1.0	1.211	1	1.211
400	3.367			844	1.196	1	1.196
221	3.122	5	3.13	553	1.174	2	1.174
122	3.065	1	3.07	943	1.149	2B	1.149
222	3.908	7	2.91	239, 12.0.0,	1.122	1B	1.122
500	2.693	1B	2.69	460, 2.0.11			
123	2.690			4.0.11, 12.1.4,	1.112	2	1.112
501	2.527	3	2.53	637			
420	2.449	5	2.45	457, 538, 157	1.087	1B	1.087
513	2.337	4	2.34	563, 165	1.072	1	1.072
602	2.252	5	2.26	13.0.3, 11.1.4,	1.054	2	1.053
600	2.244			935			
132	2.211	4	2.21	439, 662, 0.2.11	1.052		
132	2.161	2	2.16	8.2.10, 951, 265,	1.041	1	1.041
522	2.133	3	2.13	657, 663, 11.3.2			
331	2.104	2	2.11	565, 4.0.12, 944,	1.023	1B	1.023
415	2.083	1	2.08	11.4.2			
033	2.050	3	2.05	10.4.3, 172, 761,	1.000	1	1.000
306	1.992	2	1.994	955, 564, 272			
602	1.983	2	1.983	449, 067, 13.1.2,	0.980	1B	0.980
325	1.951	3	1.950	14.0.2, 14.0.3,			
522	1.934	1	1.935	10.5.0, 4.3.10	0.971	1	0.971
620	1.900	6B	1.900	0.2.12, 11.4.2,			
116	1.874	1	1.874	14.1.2, 2.0.12,	0.963	2B	0.963
603	1.817	2	1.820	14.1.3, 467,			
216	1.780	1	1.780	11.2.9	0.928	1B	0.928
041	1.766	6	1.764	12.4.2			
235	1.702	3	1.700	558, 574, 566,	0.915	1B	0.915
800	1.684			11.5.4			
334	1.658	3	1.658	649, 767, 12.3.4	0.884	1B	0.884
616	1.627	2	1.627	963, 7.0.11			
207	1.602	2B	1.602	12.5.4, 768, 281	0.876	1	0.876
227	1.579	2	1.580	871, 14.3.6, 872,			
517	1.566	1	1.566	15.1.1, 13.1.3,	0.845	0.5	0.845
326	1.550	1	1.550	13.0.10, 12.0.11			
634	1.531	2	1.530	16.1.1, 13.4.3,			
725	1.515	3B	1.515	11.4.10, 675,			
624	1.502	3B	1.502	7.5.11			
617	1.487	1B	1.487				

* Data by Honea (1961). CuK α radiation, $\lambda=1.5418$.

to and the line with large d and the strongest intensity was assumed to be $d(100)=6.81\text{\AA}$. These trial parameters were then used as input data for the computer program APPEM written by Handwerker, Appleman and Evans (see Appleman and Evans, 1967). It generates all possible spacings within the triclinic, monoclinic (there were two possibilities) and rhombic systems. However, these trial values were not successful, and so the $6.81\text{\AA}$ line was assumed to be $d(200)$ and the results seemed promising. Observed and calculated spacings were compared and indices assigned where there was a reasonable fit. These indexed reflections were subsequently used in a least-squares program for refinement of lattice constants, RSLC-3

Table 2. X-ray powder data for sklodowskite.

hkl	$d(\text{calc.}^*)\text{\AA}$	I	$d(\text{obs.}^{**})\text{\AA}$	hkl	$d(\text{cal.}^*)\text{\AA}$	I	$d(\text{obs.}^{**})\text{\AA}$
200	8.310	100	8.42	203	2.186	20	2.19
001	6.310	20	6.37	330	2.158	20	2.17
201	5.856	50	5.91	403	2.125	30	2.13
111	4.781	40	4.82	003	2.103	30	2.09
201	4.470	10	4.51	331	1.978	20	1.985
310	4.351}	40	4.33	513	1.967}	20	1.961
111	4.296}			711	1.964}		
400	4.155	80	4.19	531	1.919}	20	1.918
311	4.007	50	4.00	203	1.918}		
020	3.515	60	3.52	422	1.886	10	1.884
311	3.269}	70	3.27	911	1.852}	20	1.848
202	3.260}			602	1.846}		
221	3.014}	60	3.00	423	1.819	5	1.821
510	3.005}			023	1.805	10	1.801
312	2.863	50	2.87	912	1.768	10B	1.768
600	2.770	20	2.80	822	1.742	10B	1.740
221	2.763}	20	2.74	623	1.707	10B	1.707
112	2.724}			10.0.2	1.671	5	1.672
202	2.713	10	2.70	712	1.641	10B	1.647
420	2.684}	10	2.66	821	1.623	20	1.623
421	2.644}			333	1.594	10B	1.593
512	2.508	10	2.52	514	1.565	10	1.563
022	2.348	20	2.34	731	1.541	10	1.540
422	2.250	5	2.27				
402	2.235	20	2.22				

* $a=17.28$, $b=7.03$, $c=6.56\text{\AA}$, $\beta=105^\circ 53'$; $C2/m$ (Gorman, 1957).

** A.S.T.M. Cards No. 8-447; $\text{CuK}\alpha$ radiation, Diameter: 114.6 mm (Fron del, R. and Fron del, C., 1956).

written by T. Sakurai (1967), and the whole trial and error process repeated, in these crystal systems. The following cell parameters obtained from the final least-squares adjustment, assuming one of the monoclinic symmetry, gave the most satisfactory agreement: $a=13.73(1)\text{\AA}$, $b=7.14(1)\text{\AA}$, $c=12.35(2)\text{\AA}$, $\beta=101.2(1)^\circ$, $V=1187(3)\text{\AA}^3$, $Z=6$. $G_{\text{meas.}}=3.6$ (Fron del and Ito, 1956), $G_{\text{calc.}}=3.52(\text{OH}_2\text{O})-3.68(1\text{H}_2\text{O})$. The indexed X-ray powder data are given in Table 1.

As to the space-group, it seems appropriate to presume that boltwoodite belongs to one of the lowest symmetry space-groups in the monoclinic system, P_m , P_2 or $P2/m$, as there seems to be no extinction rule in the X-ray powder data and electron diffraction patterns. Although the longest line, $7.53\text{\AA}$ reported by Honea could

Table 3. X-ray powder data for kasolite.

<i>hkl</i>	<i>d</i> (calc.*) $\text{\AA}$	<i>I</i>	<i>d</i> (obs.**) $\text{\AA}$	<i>hkl</i>	<i>d</i> (calc.*) $\text{\AA}$	<i>I</i>	<i>d</i> (obs.**) $\text{\AA}$
001	6.500	20	6.51	$\bar{4}12$	2.477	5	2.48
110	6.163	40	6.15	212	2.474		
201	5.295	5	5.32	421	2.376	5	2.35
210	4.744	5	4.73	321	2.374		
211	4.227	60	4.21	420	2.372	20	2.18
111	4.224			230	2.199		
$\bar{3}11$	3.534	60	3.52	003	2.167	5	2.11
211	3.531			422	2.114		
202	3.252	60	3.24	222	2.112	5	2.04
002	3.250			602	2.045		
121	3.089	80	3.06	402	2.042	5	1.966
021	3.088			113	1.970		
220	3.082	100	2.92	$\bar{6}12$	1.963	20	1.879
410	2.926			412	1.961		
221	2.926	5	2.74	223	1.883	5	1.829
121	2.924			123	1.883		
312	2.743	5	2.65	$\bar{6}21$	1.871	20	1.741
112	2.741			620	1.831		
321	2.664	5	2.65	431	1.749	20	1.741
221	2.662			140	1.739		
402	2.647						
202	2.644						

* $a=13.31$, $b=7.02$, $c=6.72\text{\AA}$, $\beta=104^\circ42'$; $P2_1/a$ (Mokeyeva, 1964).

** Mineraux d'Uranium du Haut Katanga (Musée Royal du Congo Belge, Tervuren) (1958). Diameter: 240 mm. A.S.T.M. Cards No. 12-210.

not be indexed, this one may be suspicious one as this line does not exist in the data of Frondel and Ito nor in the data for the synthetic boltwoodite-like materials discussed by Honea.

Frondel and Ito, and Honea point out that there is a resemblance of the X-ray powder pattern to those of sklodowskite and kasolite. This resemblance seems due to the similarity among these minerals in cell dimensions and (probably) their structures.

The newly indexed X-ray powder data for sklodowskite and kasolite are also given in Tables 2 and 3 as it seems that there is no wholly indexed data for these minerals available.

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