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X-ray powder data for caledonite

IN our paper dealing with the crystal structure of caledonite (C. Giacobazzo, S. Menchetti, and F. Scordari, *Acta Cryst.* **B29**, 1986–90, 1973), lattice parameters refined from a zero-level Weissenberg and a powder photograph were reported; powder data,

TABLE I. *Indexed powder data and unit-cell parameters of caledonite*

<i>hkl</i>	<i>d</i> _{calc}	<i>d</i> _{obs}	<i>I</i>	<i>hkl</i>	<i>d</i> _{calc}	<i>d</i> _{obs}	<i>I</i>	<i>hkl</i>	<i>d</i> _{calc}	<i>d</i> _{obs}	<i>I</i>
101	6.24 Å	6.24 Å	15	421	2.661 Å	2.661 Å	21	023	1.866 Å	1.866 Å	19
400	5.02	5.02	8	412	2.564	2.564	10	631	1.861	1.861	53
310	4.88	4.88	7	800	2.511	2.510	7	223	1.834	1.834	3
011	4.83	4.83	12	521	2.473	2.473	9	730	1.834		
111	4.70	4.69	57	122	2.399	2.399	14	432	1.798	1.798	4
301	4.69			030	2.381	2.383	2	323	1.798		
211	4.35	4.35	3	130	2.365	2.364	10	912	1.786	1.786	14
311	3.92	3.92	5	602	2.344	2.345	3	040	1.786		
020	3.57	3.57	24	621	2.289	2.288	9	613	1.775	1.775	7
120	3.52	3.51	5	322	2.273	2.273	31	423	1.749	1.749	3
510	3.50	3.50	3	330	2.244	2.242	10	703	1.738	1.738	5
501	3.427	3.426	19	612	2.227	2.226	36	532	1.738		
600	3.348	3.348	8	422	2.178	2.175	9	041	1.723	1.723	12
002	3.282	3.282	24	103	2.175			10.0.2	1.713	1.713	2
320	3.151	3.152	36	910	2.130	2.130	24	11.1.1	1.708	1.708	2
021	3.137	3.139	100	303	2.080	2.079	11	10.2.1	1.691	1.691	3
511	3.090	3.090	12	522	2.071	2.070	10	523	1.691		
610	3.032	3.031	55	530	2.048	2.048	9	713	1.691	1.683	5
221	2.995	2.994	5	213	2.048			440	1.683		
012	2.982	2.983	5	431	2.044	2.044	9	12.0.0	1.674	1.674	12
212	2.859	2.858	9	911	2.026	2.028	21	632	1.668	1.668	26
321	2.841	2.840	7	821	1.960	1.959	3	341	1.668		
611	2.752	2.752	43	622	1.960			10.1.2	1.688		
312	2.724	2.727	3	503	1.922	1.918	10				
520	2.669	2.675	14	132	1.919						

Unit-cell parameters (data of Giacobazzo *et al.*, 1973, in parentheses): *a* 20.088 ± 0.002 (20.089 ± 0.007), *b* 7.143 ± 0.001 (7.146 ± 0.003), *c* 6.564 ± 0.001 (6.560 ± 0.005)

however, were not given. Since there are some differences from ASTM 8–153 (PDS-1971) and since the J.C.P.D.S. has asked us for powder data we feel that this note may be useful. A new and more accurate diffractometer trace was obtained, using Cu-K α radiation and NaF as internal standard, from 14° to 57° 2 θ at a scanning speed of 0.125°/min; 49 indexed peaks were used for the least-squares refinement of the unit-cell dimensions. Calculated and observed *d*-spacings and estimated intensities are presented in Table I, together with the unit-cell dimensions derived.

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