SHORT COMMUNICATIONS

X-ray and other data for mellite[1]

In 1933 T. F. W. Barth and C. J. Ksanda published X-ray crystallographic data for mellite, $Al_2C_{12}O_{12}.18H_2O$, but did not include X-ray powder data; these are now provided, together with a partial chemical analysis, and some observations on fluorescence in ultra-violet light.

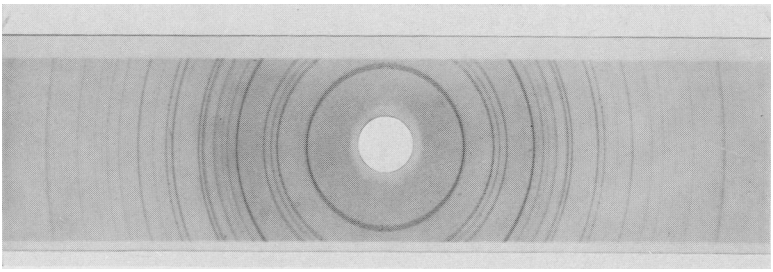

Fig. 1. X-ray powder photograph of mellite. Co-$K\alpha$ radiation, 11·46 cm diameter camera.

Most of the work was carried out on specimens from Artern (51° 23′ N., 11° 17′ E.), East Germany (G.S.M. no. MI. 21762). The refractive indices obtained from the smooth faces of a pyramidal crystal (1 cm along its longer edge) using a Rayner refractometer (calibrated to give an accuracy $\pm 0{\cdot}001$) and sodium light were $\epsilon = 1{\cdot}512$ and $\omega = 1{\cdot}540$. The specific gravity, determined by hydrostatic weighing in toluene and corrected for temperature, was 1·606.

X-ray powder films were taken of material from Artern and from Malevka (53° 36′ N., 38° 16′ E.), Tula, USSR (G.S.M. Ludlam collection no. 10913). Both specimens gave identical patterns. The X-ray powder data (table I) were obtained from diffractometer traces of the Artern material, lead nitrate being used as an internal standard. All the diffraction lines were satisfactorily indexed on a tetragonal cell of dimensions a 21·91 Å, c 23·20 Å, giving an axial ratio $c/a = 1{\cdot}059$. These cell dimensions are in good agreement with the values a 22·0 kX, c 23·3 kX, $c/a = 1{\cdot}059$ obtained by Barth and Ksanda from single crystal rotation photographs. Barth and Ksanda concluded that the space group is

almost certainly either $P4_122$ or $P4_322$, and the data listed here are compatible with this conclusion.

There are sixteen formula units in the unit cell. The specific gravity 1·606 determined on the Artern material is less than the specific gravity

TABLE I. X-ray powder data for mellite from Artern, East Germany (G.S.M. no. MI. 21762) from diffractometer charts taken with Cu-$K\alpha$ radiation at a scanning speed of $\frac{1}{8}°$ 2θ/min. Lead nitrate (a 7·8568 Å) was used as an internal standard. Indexed on a unit cell having: a 21·91 Å, c 23·20 Å. The intensities are relative peak heights.

hkl	d_{obs}	d_{calc}	I/I_1	*hkl*	d_{obs}	d_{calc}	I/I_1
202	7·99 Å	7·97 Å	100	901		2·421	
220	7·77	7·75	7	910	2·422 Å	2·420 Å	4
004	5·80	5·80	55	753		2·419	
400	5·49	5·48	22	911	2·405	2·406	11
330	5·16	5·164	40	518		2·404	
313		5·160		419	2·317	2·319	6
422	4·52	4·513	2	1.0.10		2·307	
511	4·23	4·225	70	339	2·306	2·306	8
404	3·99	3·982	19	825		2·306	
225		3·980		931	2·299	2·298	4
334	3·86	3·857	8	932	2·266	2·265	6
315		3·855		509,439	2·220	2·222	3
531	3·72	3·709	8	548	2·212	2·212	6
325	3·69	3·688	17	3.0.10		2·211	
504,434	3·49	3·496	14	771	2·206	2·203	3
415		3·495		772	2·175	2·174	4
443	3·46	3·463	30	10.1.1	2·171	2·171	2
226		3·460		10.2.0	2·149	2·149	2
541	3·39	3·385	30	4.1.10	2·126	2·126	2
444	3·22	3·221	< 1	539		2·126	
604	3·083	3·089	5	951	2·119	2·119	2
711	3·077	3·071	4	648		2·098	
551		3·071		4.2.10	2·097	2·097	9
721	2·985	2·985	25	619		2·096	
544	2·952	2·947	1	952	2·093	2·093	6
703	2·900	2·901	20	827	2·073	2·073	1
008		2·900		639	2·024	2·024	2
800	2·739	2·739	8	961	2·019	2·0179	1
733	2·697	2·696	2	3.1.11		2·0176	
705	2·598	2·595	9	963		1·9594	
660	2·582	2·582	22	6.0.10	1·959	1·9581	3
803		2·582		729		1·9578	
752	2·491	2·488	1	767,927	1·932	1·9323	6
607	2·456	2·454	2	838	1·921	1·9210	12
				776		1·9209	
				971,11.3.1	1·916	1·9151	11

1·704 calculated on the assumption that the formula is $Al_2C_{12}O_{12}\cdot 18H_2O$. However, the published analyses (Doelter, 1931, and Hintze, 1933) of natural material show less water than would be expected if there are $18H_2O$ in the formula, and the observed specific gravity corresponds to a water content of $15{\cdot}7H_2O$.

A partial chemical analysis was carried out. On heating at 105° C for two days a loss in weight equivalent to $10{\cdot}7_5$ molecules of water was

recorded, assuming an original molecular water content of 15·7, and the material no longer yielded an X-ray pattern.

Ignition of 0·1089 g of the material in a platinum crucible over a Meker burner gave a residue shown by X-ray examination to consist of several phases of alumina, Al_2O_3, corresponding in weight to 8·01(8) % of aluminium in the mineral, equivalent to 15·70 molecules of water in the formula $Al_2C_{12}O_{12}.xH_2O$.

Microchemical gravimetric carbon determinations were carried out by heating a few milligrams of the mineral in a closed, evacuated vessel with a chromic-phosphoric acid mixture, the evolved carbon dioxide being absorbed in baryta solution and subsequently weighed as barium carbonate. Three determinations for total carbon (21·3 %, 22·3 %, and 22·0 %) were carried out. One (21·3 %) is in fair agreement with that (21·42 %) calculated from the aluminium figure obtained by ignition; the higher values are probably due to the presence of undetected inclusions of free carbonaceous matter in the mineral.

A series of specimens was examined under long-wave (3650 Å) and short-wave (2537 Å) ultra-violet light. Material from Artern showed a whitish-yellow fluorescence, the intensity varying from very strong to weak under 3650 Å radiation and from moderate to weak under 2537 Å radiation. Specimens from Malevka, Tula, USSR, were not obviously fluorescent. The blue fluorescence described in Dana's 'System of Mineralogy', 7th edition, was not observed.

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[1] Published by permission of the Director, Geological Survey and Museum, and of the Government Chemist.

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Calzirtite and associated minerals from Tapira, Brazil

IN 1961 Zdorik, Sidorenko, and Bykova described a new calcium titano-zirconate, which they named calzirtite, found in a metasomatic