Acta Cryst. (1965). **19**, 1059

Crystal data for scandium molybdate, $Sc_2(MoO_4)_3$.

By A. W. BIEDL*, *Department of Geological Sciences, Harvard University, Cambridge, Mass., U.S.A.*

(*Received* 12 *April* 1965 *and in revised form* 1 *June* 1965)

Single crystals of scandium molybdate were grown in lithium molybdate melts by cooling from 1150 to 750 °C. The crystals are pseudotetragonal platelets and range in size up to several millimeters. They exhibit excellent cleavage on (001). The optical properties are: $n\alpha = 1{\cdot}798$, $n\beta = 1{\cdot}820$, $n\gamma = 1{\cdot}826$, $2V\alpha = 65°$ (calculated). The vibration direction corresponding to $n\alpha$ is parallel to the c axis. The density has been determined by means of the Berman microbalance on a polycrystalline sample: 3·08 g.cm^{-3}. X-ray fluorescence analysis showed scandium and molybdenum only.

Precession photographs were made with filtered molybdenum radiation (0·71069 Å). The following lattice constants were found: $a = 9{\cdot}66$, $b = 9{\cdot}56$, $c = 13{\cdot}25$ Å, all $\pm 0{\cdot}03$ Å. The conditions $0kl$, $k+l=2n$; $h0l$, $h=2n$; $hk0$, $k=2n$ determine the space group as *Pnab* (D_{2h}^{14}). (The setting of *International Tables for X-ray Crystallography* is *Pbcn*; the setting adopted here keeps the pseudotetragonal axis as c axis). Powder photographs have been made with filtered copper radiation (Table 1). The values under $d_{obs}{}^N$ in Table 1 were measured carefully with a Norelco diffractometer, quartz being used as internal standard. (The lattice constants for quartz have been assumed as $a_0 = 4{\cdot}91331$, $c_0 = 5{\cdot}40488$ Å; measurements were made at room temperature.)

Refinement with the LCLSQ-program on the IBM 7094 computer yielded the following lattice constants: $a = 9{\cdot}641 \pm 0{\cdot}005$, $b = 9{\cdot}550 \pm 0{\cdot}004$, $c = 13{\cdot}246 \pm 0{\cdot}005$ Å. With a cell content of $4Sc_2(MoO_4)_3$, the calculated density is 3·103 g.cm^{-3}.

Nassau, Levinstein & Loiacono (1964) have announced the compound $Sc_2(WO_4)_3$ with $a = 13{\cdot}2$, $b = 9{\cdot}64$, $c = 9{\cdot}46$ Å, space group D_{2h}^{14}. Except for the interchange of axes, these dimensions correspond to those of scandium molybdate; it is very probable that the two compounds are isostructural. (A synthesis of $Sc_2(WO_4)_3$ has also been reported by Borisenko & Komissarova (1960), but no details are given).

A further investigation of this scandium molybdate is not intended.

I wish to acknowledge the constant encouragement of Dr C. Frondel. The refinement program LCLSQ, written by Dr Charles W. Burnham, was made available by D. R. Waldbaum. This study is supported by the Advanced Research Project Agency contract SD-88.

References

NASSAU, K., LEVINSTEIN, H. J. & LOIACONO, G. M. (1964). *J. Amer. Ceram. Soc.* **47**, 364.

BORISENKO, L. F. & KOMISSAROVA, L. N. (1960). *Dokl. Akad. Nauk SSSR*, **135**, 430.

* Present address: Institut für Mineralogie, Lehrstuhl für Kristallographie, Ruhr-Universität Bochum, Germany.

Table 1. *Powder photographic data for* $Sc_2(MoO_4)_3$, Cu $K\alpha$ (1·54178 Å), *Ni filter, camera diameter* 114·6 *mm, Straumanis arrangement.*

The values under $d_{obs}{}^N$ were measured on a Norelco diffractometer with quartz as internal standard. Intensities estimated visually.

No.	I	d_{obs}	$d_{obs}{}^N$	d_{calc}	hkl
1	3	6·7	6·62	6·623	002
2	6	6·0	6·04	6·038	111
3	1	4·76		4·775 4·739	020 112
4	7	4·55	4·529	4·530	201
5	8	4·29	4·278	4·279	120
6	10	4·10	4·093 4·075	4·093 4·072	211 121
7	10	4·01	4·007	4·008	013
8	2	3·90		3·899 3·873	202 022
9	3	3·71	3·703	3·701	113
10	8	3·61		3·608 3·594	212 122
11	5	3·398	3·391	3·392	220
12	1	3·310		3·313	004
13	1	3·284		3·286	221
14	6	3·095		3·095 3·082 3·073	031 213 123
15	2	3·023		3·019	222
16	4	2·974		2·976 2·968	114 311
17	<1	2·831		—	Sc_2O_3
18	8*b*	2·751		2·767 2·750 2·729 2·721	312 132 204 024
19	1	2·679		2·690 2·666	223 320
20	2	2·622		2·624 2·619 2·614	214 124 321
21	1	2·560		2·553	015
22	5	2·496		2·494	133

plus numerous lines at higher angles.