## A RHOMBOHEDRAL POLYTYPE OF MOLYBDENITE\*

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Rhombohedral molybdenite (molybdenite-3R) has been identified as an accessory mineral in quartz-feldspar porphyry occurring at the Con mine, Yellowknife, District of Mackenzie. The following observations on the occurrence and origin of the quartz-feldspar porphyry have been taken from Boyle (1961).

Irregular dyke-like bodies of quartz-feldspar porphyry are found in the underground workings of the Con, Negus and Rycon mines. The porphyries contain phenocrysts of quartz and zoned plagioclase in a groundmass of fine-grained plagioclase, quartz, microcline, muscovite, carbonates and chloritized biotite. Pyrite and pyrrhotite are particularly abundant in the porphyries in the vicinity of the Con mine, and molybdenite is present as disseminated flakes in a few of the bodies. Other accessory minerals include small amounts of apatite, zircon, rutile and epidote. The sulphides appear to be primary constituents, and probably crystallized with the quartz and feldspar, because they fill interstices between these minerals and form along the cleavage planes of biotite.

The origin of the porphyry dykes and masses is an enigma requiring further research. On the one hand the porphyries present metasomatic features and may have formed from processes of metamorphic differentiation. This is borne out by the facts that some contain an abundance of sulphides and carbonates and are enriched in chromium, features foreign to granitic rocks. On the other hand they display sharp contacts, are dyke-like, and as regards their major components, have a similar composition to the western granodiorite. This suggests that they may have originated either by magmatic or granitization processes. The latter seems to fit the facts best and the author is of the opinion that the porphyries represent concentrations of various elements mobilized during granitization at depth.

The present writer has examined x-ray powder diffraction patterns of molybdenites from three different types of occurrences in the Yellowknife district. Molybdenites from a pegmatite associated with the Prosperous Lake granite and from a quartz lens in a shear zone of the Crestaurum system give x-ray patterns in close agreement with the standard pattern of common hexagonal molybdenite. The x-ray pattern of molybdenite from the Con quartz-feldspar porphyry shows very distinct differences, most noticeable of which are the absence of the (10.2) reflection and presence of strong doublets at the reflecting positions of the (10.3) and (10.5) planes of normal molybdenite. These differences have been noted

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by Bell & Herfert (1957) and Zelikman et al. (1961) on patterns of synthetic rhombohedral molybdenum disulphide.

Bell & Herfert (1957) have shown that the synthetic material has rhombohedral symmetry, space group  $R3m-C_{3c}^{5}$ , with the *a* axis identical to that of hexagonal MoS<sub>2</sub> and the *c* axis 1.5 times larger. The CdCl<sub>2</sub>-type structure proposed by Bell & Herfert has been refuted by Jellinek *et al.* (1960) on the grounds that it is incompatible with the *x*-ray diffraction data. The latter authors show that the structure can be described as: 3 Mo in 3(*a*), with z = 0; 3 S in 3(*a*), with  $z \approx \frac{1}{4}$ ; and 3 S in 3(*a*) with  $z \approx 5/12$ . Zelikman *et al.* have reported the possible existence of several structural modifications of synthetic MoS<sub>2</sub> which may result from alternating combinations of hexagonal and rhombohedral packing.

X-ray diffraction data for rhombohedral molybdenite from the Con mine are listed in Table 1 and compared with hexagonal molybdenite from the Yellowknife area. The patterns were taken with a 57.3 mm.

	Mo Yeli	olybdenite lowknife dis P6./mmc	-2H strict	Molybdenite3R Con Mine R3m				
a = 3.16, c = 12.28Å				a = 3.16, c = 18.33Å				
I	d(meas.)	d(calc.)	hk.l	I	d(meas.)	d(calc.)	hk.l	
10	6.01	6.14	002	10	6.09	6.11	003	
ĩ	3.04	3.07	004	ĩ	3.04	3.06	006	
2	2 73	2 74	ĩõõ	7	2 71	2.71	101	
ĩ	2 66	2 67	101	ė	2 63	2 62	012	
1	2 50	2.50	102	v	4.00	2.02	012	
Т	2.00	2.00	102	6	2 344	2 349	104	
Q	9 97	9 975	103	0	2.011	2.010	101	
0	2.21	2.210	100	ß	9 104	2 103	015	
1	9.04	9.045	104 008	2	9 024	2.130	000	
I	2.04	2.040	104,000	0 4	1 004	1 809	107	
=	1 00	1 000	105	4	1.009	1.094	101	
Э	1.82	1.828	105	9	1 725	1 757	010	
т	1.04	1 000	100	ð	1.700	1.707	010	
2	1.04	1.639	106	-	1 801	1 500	110	
2	1.58	1.580	110	<u> </u>	1.581	1.580	110	
3	1.53	1.532	008, 112	7	1.529	1.529	00.12, 113	
12	1.48	1.477	107	_			~	
				$\frac{1}{2}$	1.426	1.423	01.11	
				12	1.403	1.403	116	
12	1.36	1.360	201	<b>2</b>	1.363	1.364	021	
-				1	1.357	1.353	202	
븕	1.337	1.337	202, 108					
-			,	1	1.313	1.311	024	
1	1.297	1.298	203	1	1.283	1.282	205	
1	1.251	1.251	204.116	4	1.249	1.248	119	
ī	1 226	1 228	00 10	ī	1 225	1.222	00.15	
1	1.220	1.221	109	ĩ	1.214	1.213	027	
12	1 195	1 195	205	1	1 179	1.181	01.14	
1	1 101	1 101	118	5	1 000	1 098	11 12 02 10	
т	1.101	1.101	110	1	1 057	1 057	10 16 20 11	
				2	T.001	1.001	10.10, 40.11	

TABLE 1. X-RAY POWDER DATA FOR MOLYBDENITE POLYTYPES

Molybdenite-2H Yellowknife district $P6_3/mmc$ $a = 3.16, c = 12.28\text{\AA}$					Molybdenite3 $R$ Con Mine R3m a = 3.16, c = 18.33Å				
I	d(meas.)	d(calc.)	hk.l	I	d(meas.)	d(calc.)	hk.l		
1	1 034	1 034	10 11 210	1	1 031	1 030	211, 122		
1	1 021	1 021	208 212	22	1 017	1 018	0018		
2	1.021	1.041	200, 212	2	1 000	1 009	214		
1	1 009	1 003	919	5	0.006	0.005	125		
1	1.002	1.005	410	1	0.990	0.000	02 13		
1	0.060	0.070	11 10	20	0.901	0.982	11 15		
2	0.909	0.970	11.10	1	0.900	0.901	917		
т	0.059	0.059	91 E	Т	0.904	0.902	211		
T	0.900	0.999	210	1	0.045	0.048	20 14		
1	0.019	0.019	200 00 10	1	0.940	0.940	20.14		
2	0.913	0.913	300, 20.10	0	0.919	0.912	000 000 01 10		
2	0.902	0.902	302	2	0.902	0.902	303, 21.10		
1	0.894	0.893	10.13						
12	0.877	0.877	00.14	12	0.879	0.879	02.16, 12.11		
				$\frac{1}{2}$	0.874	0.874	00.21,306		
1	0.865	0.865	20.11						
				12	0.855	0.856	11.18		
				$\frac{1}{2}$	0.848	0.847	20.17		
<u></u>	0.836	0.835	10.14	-					
Ĩ	0.834	0.833	306	<b>2</b>	0.834	0.833	309, 21.13		
ĩ	0.790	0.790	$220.\ 21.10$	<b>2</b>	0.791	0.790	220		
3	0.784	0.784	222, 308	5	0.784	0.783	223, 30.12		
$\tilde{2}$	0.778	0.777	20.13				•		
-									

TABLE 1 (Concluded)

diameter Norelco camera and nickel-filtered copper radiation. The indexing based on unit cell dimensions a = 3.16 and c = 18.33 is consistent with space group R3m. A spectrographic analysis of the mineral showed Mo as the only major constituent; minor amounts of Si, Fe and Al, and a trace of Mg, were reported.

Because of the possibility that other polytypes may be discovered it is proposed that the system of nomenclature introduced by Ramsdell (1947) for SiC, and later adopted for wurtzite, also be used for molybdenite. Following this system, the common hexagonal polytype is designated molybdenite-2H and the new polytype from the Con mine is designated molybdenite-3R.

## REFERENCES

BELL, R. E., & HERFERT, R. E. (1957): Preparation and characterization of a new crystalline form of molybdenum disulphide, J. Am. Chem. Soc., 79, 3351-3354.

BOYLE, R. W. (1961): The geology, geochemistry, and origin of the gold deposits of the Yellowknife district, Geol. Surv. Canada, Mem., 310.

JELLINEK, R., BRAUER, G., & MÜLLER, H. (1960): Molybdenum and niobium sulphides, Nature, 185, 376.

RAMSDELL, L. S. (1947): Studies on silicon carbide, Am. Mineral, 32, 64-82.

ZELIKMAN, A. N., CHISTYAKOV, YU.D., INDENBAUM, G. V., & KREIN, O. E. (1961): Crystal structure analysis of MoS<sub>2</sub> synthesized by various methods; *Kristallografiya*, 6, No. 3, 389-94.

Manuscript received June 18, 1962