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McGILLITE, A NEW MANGANOUS HYDROXYCHLOROSILICATE

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ABSTRACT

Found in 1945 in the Sullivan mine at Kimberley, B.C., long mistaken for friedelite, mcGillite occurs as fracture fillings in Middle Proterozoic sediments, together with sphalerite, boulangerite, galena, jamesonite and milky quartz. It is anhedral, light to dark pink, with pearly lustre, easy and good cleavage {0001}, and difficult but fair cleavages {10$\bar{1}$1}. The Vickers hardness ranges from 278 to 330 kg/mm². The formula obtained on the microprobe, $(Mn^{2+}_{6.95}Fe^{2+}_{0.63}Mg_{0.42})_{\Sigma=8.00}(Si_{5.93}Fe^{3+}_{0.07})_{\Sigma=6.00}[O_{14.94}(OH)_{8.21}Cl_{1.85}]_{\Sigma=25}$, approximates $Mn_8Si_6O_{15}(OH)_8Cl_2$. The cell dimensions *a* 13.498(3) and *c* 85.657(15) Å (at 21°C, for λAg *Ka*=0.5609 Å), with *Z*= 24, lead to *Dx*= 3.071 against *Dm*= 2.98(4) g/cm³ (Berman balance, 21°C). Laue class $\bar{3}m$ and systematic extinctions indicate *R*3*m* or *R*$\bar{3}$*m*. The pyroelectric test is negative. The refractive indices (Na*D* light, 21°C) are: n_ω = 1.6685(15), n_ϵ = 1.6415(15). McGillite belongs to the pyrosmalite group, but shows considerable stacking disorder. The common pseudorepeat *c'* ~ 7.16 Å here equals *c*/12. The layer thickness, 4*c'* = *c*/3, is required by the *R* lattice. The powder X-ray pattern, controlled by Mn contributions, is so similar to that of friedelite that it has little diagnostic value, but any single-crystal diffraction pattern reveals intense diffuse rods parallel to *c**. A *c*-axis rotation pattern uniquely characterizes mcGillite. The name honors McGill University.

Keywords: manganous hydroxysilicate, pyrosmalite group, new mineral, disordered crystal structure, mcGillite.

SOMMAIRE

Découverte en 1945 à la mine Sullivan de Kimberley (C.B.) et longtemps prise pour friedelite, la mcGillite constitue un remplissage de cassures dans des roches sédimentaires du Protérozoïque moyen, avec sphalérite, boulangérite, galène, jamesonite et quartz laiteux. Allotriomorphe, d'un rose plus ou moins foncé, d'éclat nacré, elle montre un clivage facile et bon {0001} et trois clivages difficiles mais nets {10$\bar{1}$1}. Dureté Vickers: 278 à 330 kg/mm². La formule que donne la microsonde, $(Mn^{2+}_{6.95}Fe^{2+}_{0.63}Mg_{0.42})_{\Sigma=8.00}(Si_{5.93}Fe^{3+}_{0.07})_{\Sigma=6.00}[O_{14.94}(OH)_{8.21}Cl_{1.85}]_{\Sigma=25}$, est proche de $Mg_8Si_6O_{15}(OH)_8Cl_2$. Les dimensions de maille, *a* 13.498(3), *c* 85.657(15) Å (à 21°C, λAg*Kα* = 0.5609, pour *Z* = 24, mènent à *Dx* = 3.071, contre *Dm* = 2.98(4) (balance Berman, 21°C). La classe de Laue $\bar{3}m$ et les extinctions systématiques donnent *R*3*m* ou *R*$\bar{3}$*m;* l'essai pyroélectrique est négatif. Les indices de réfraction (Na*D*, 21°C) sont: n_ω = 1.6685(15), n_ε = 1.6415(15). La mcGillite fait partie du groupe de la pyrosmalite, mais avec grand désordre d'empilement. La pseudo-période commune *c'* ~ 7.16 Å est ici égale à *c*/12. L'épaisseur de la couche, 4*c'* = *c*/3, est celle que requiert le mode *R*. Le cliché de poudre, dominé par Mn, simule celui de la friedelite et n'est guère diagnostique; tout cliché de cristal unique révèle d'intenses traînées diffuses parallèles à *c**. Une photo de cristal tournant (axe *c*) caractérise la mcGillite. Dédiée à l'Université McGill.

Mots-clés: hydroxysilicate de manganèse, groupe de la pyrosmalite, nouvelle espèce, structure cristalline désordonnée, mcGillite.

INTRODUCTION

In 1945 a pink mineral occurring as open-space fracture fillings was found in a development raise in the southwest part of the orebody, at the Sullivan mine, Kimberley, B.C. The raise was located near the Cleaver fault in an area where both ore and enclosing sedimentary rocks are highly manganiferous; this area is now an open pit, and the pink mineral is no longer to be found. Tentatively identified as friedelite, the mineral was considered of sufficient interest to warrant the storage of many hand specimens, all containing the mineral in small amounts (mostly less than 2%, occasionally 3 to 7% by volume). No other occurrences have been recorded in the mine.

Thirty-one years later, one of us (M.B.) held a summer job at the Sullivan mine and was presented with one of the historic hand specimens by Mr. Robert O'Brien, then Senior Geologist at the mine. A routine X-ray check was made at McGill University to confirm the determination of the mineral as friedelite, by taking a rotation pattern about the normal to the prominant cleavage plane. Contrary to expectation, the translation repeat was found to be 85.7 Å, four times the value for the corresponding direction in friedelite. Further work convinced us that we were dealing with a new mineral, the fifth member of the pyrosmalite group which already includes manganpyrosmalite, schallerite and friedelite. The name mcGillite honors McGill University for its pioneering role in Canadian geology and its 150 years of distinguished service to Canada, Québec and Montréal. The mineral, its name and spelling were approved by the I.M.A. Commission on New Minerals and Mineral Names on June 5, 1979. Type material is deposited with the National Mineral Collection, Geological Survey of Canada, Ottawa, and with the Redpath Museum, McGill University, Montréal. The Royal Ontario Museum, the Smithsonian Institute and the British Museum received mcGillite specimens directly from Cominco Limited.

A second locality for mcGillite has already been found (Y. Takéuchi, priv. comm., April 27, 1979) at the Kyurazawa mine, Tochigi Prefecture, Japan.

GEOLOGICAL SETTING AND ASSOCIATED MINERALS

The orebody of the Sullivan mine is up to 100 m thick and is conformable with Middle Proterozoic sedimentary rocks belonging to the Lower and Middle Aldridge Formation of the Purcell Supergroup. Although the immediate footwall of the orebody consists of intraformational conglomerates throughout much of the mine area, the footwall consists mainly of fine-grained, rhythmically graded beds of impure quartzite and argillite; the hanging wall consists of thicker, more arenaceous beds.

Structurally the orebody occurs in a wide, north-plunging anticline. During greenschist-facies metamorphism, the fine fraction of the original rock recrystallized, but the coarser material remained unaffected. The hanging-wall sedimentary units are albitized and locally chloritized and tourmalinized. The footwall sedimentary rocks are heavily tourmalinized. The central and northern portions of the orebody are underlain by discontinuous north-trending zones of coarsely brecciated rocks extending downward to unknown depths. The orebody is bounded by two north-dipping steep normal faults, Hidden Hand and Kimberley; the latter, just north of the orebody, has a stratigraphic displacement of 3,300 m. The orebody is transected by a set of radiating steep normal faults striking from NE to NW and dipping roughly eastward (Freeze 1966).

In the orebody, pyrrhotite, sphalerite, galena and pyrite are the principal sulfides; boulangerite, chalcopyrite and arsenopyrite occur in minor proportions, whereas magnetite, jamesonite and tetrahedrite have been identified only in small amounts. The iron sulfides, predominantly pyrrhotite and pyrite, constitute a core near the centre of the deposit (Freeze 1966). East-southeast of this iron sulfide core lies a domal structure around which the non-iron sulfides are arranged concentrically. The Pb/Zn ratio is highest close to the dome and decreases outward.

McGillite is most often associated with very dark sphalerite and small amounts of boulangerite, galena, jamesonite and milky quartz. The extent of the fractures containing mcGillite is unknown (D.T. Bishop, priv. comm., Jan. 4, 1979). Probably no other pyrosmalite-group mineral is present in the mine; at least, none has been detected in any of the specimens studied by single-crystal X-ray techniques, in spite of an intensive search.

CHEMICAL COMPOSITION

The small amount of mcGillite available for study precluded wet-chemical analysis. We did, however, heat grains of mcGillite in a closed tube: the grains turned dark brown and gave off water that condensed at the cool end of the tube. We also dropped some cold 6*N* HCl on a mc-

TABLE 1. CHEMICAL ANALYSES OF PYROSMALITE-GROUP MINERALS

Mineral: Analyst:	McGILLITE W.H.MacLean	FRIEDELITE W.T.Schaller	SCHALLERITE L.H. Bauer	MANGAN-PYROSMALITE L.H. Bauer	PYROSMALITE F.Zambonini
SiO_2	34.54	34.69	31.44	34.13	34.71
As_2O_3	<0.1	not det.	12.24	0.13	Al_2O_3 0.26
MnO	47.76	48.00	44.70	39.09	24.30
FeO	4.85	1.45	2.12	12.43	27.76
MgO	1.62	0.98	2.19	0.74	1.11
ZnO	<0.1	1.05	0.54	1.94	not det.
CaO	<0.05	0.63	0.36	nil	0.43
Cl	6.36	3.43	0.08	3.80	4.16
H_2O+	7.16*	9.08	6.55	8.18	8.31
H_2O^-	not det.	1.94	not det.	not det.	not det.
	102.29	101.25	100.22	100.44	101.04
O=Cl	1.44	0.77	0.02	0.86	0.94
Total	100.85	100.48	100.20	99.58	100.10

NUMBER OF IONS ON THE BASIS OF SIX TETRAHEDRALLY COORDINATED CATIONS

Si	5.93	6.00	5.86	5.99	5.95
Fe^{3+}	0.07	-	0.14	As 0.01	Al 0.05
			As 1.38		
Mn^{2+}	6.95	7.03	7.06	5.81	3.53
Fe^{2+}	0.63	0.21	0.19	1.82	3.98
Mg	0.42	0.25	0.61	0.19	0.28
Zn	-	0.13	0.07	0.25	-
Ca	-	0.12	0.07	nil	0.08
Cl	1.85	1.01	0.03	1.13	1.21
OH	8.21*	10.47	8.14	9.57	9.50

*Calculated on the basis of 25 anions per formula unit. McGILLITE from Sullivan Mine, Kimberley, B.C. Present work. FRIEDELITE from Buckwheat Mine at Franklin, N.J., Catalogue No. 87123. Wet chemical analysis reported in Bauer & Berman (1928); Table 1, No. 3. MANGANPYROSMALITE from Sterling Hill, N.J. Wet chemical analysis in Frondel & Bauer (1953); Table 2. SCHALLERITE from Franklin, N.J., type material. Wet chemical analysis in Bauer & Berman (1928); Table 1, No. 7. Recalculated on the basis of 14 cations, exclusive of As which is assumed to form an addition solid solution. PYROSMALITE from the Bjulke mine, Nordmark. Wet chemical analysis, Zambonini (1901).

Gillite chip: small bubbles were thus liberated while the crystal decomposed without gelatinizing. We infer that the $Mn(OH,Cl)_2$ layer is attacked by HCl, which leads to a breakdown of the crystal structure. An electron-microprobe analysis, in which all atoms heavier than Fe were looked for but not found, was carried out by Professor W.H. MacLean at McGill University. Another probe analysis was performed by Mr. C. Hadidiacos at the Geophysical Laboratory of the Carnegie Institution of Washington, Except for the weight percentage of chlorine, for which a standard with too low a chlorine content was used, the latter's results show overall agreement with those of Professor MacLean, whose analysis is compared with the wet-chemical analyses of the other four members of the pyrosmalite group (Table 1). The empirical formulae are based on six tetrahedrally coordinated cations, namely Si and small amounts of Fe^{3+} Al or As, so as to make the sum of octahedrally coordinated cations equal to eight within the accuracy of the analyses. In schallerite we assume that the arsenic atoms do not substitute for Mn in the brucite-type layers of the crystal structure. Hey (1962) suggested this structural interpretation of schallerite analyses when he proposed the formula $(Mn,Fe)_8As_{2-2x}Si_6(O,OH,Cl)_{26}$ with $0.6 \leq x \leq 1.2$. The cations of the brucite-type layers consist of Mn^{2+}, Fe^{2+}, Mg, Zn and Ca, with only the first three detected in mcGillite. In the latter we must also assume 25 anions *per* formula unit, so as to be able to calculate the hydroxyl-ion content.

The unique chemical feature of mcGillite consists in its high chlorine content, 18.5 at. % of the univalent anions in the structure. Since random substitution of Cl^- for OH^- in minerals is rare, if not unproved, we shall consider only the idealized formula $(Mn,Fe,Mg)_8Si_6O_{15}(OH)_8Cl_2$. With $Z = 24$ it requires a total of 48 chlorine ions *per* cell, which can be distributed, in space group $R\bar{3}m$, among three 18-fold (h) positions of site symmetry m and occupancy 8/9. Thus we expect Mn in three out of four brucite-type layers to be coordinated to Cl atoms. McGillite cannot, therefore, be considered a polytype of the other members of the pyrosmalite group; it might be called a polytypoid, according to the Report of the IMA–IUCr Joint Committee on Nomenclature (Bailey 1978). It is as chemically distinct as is schallerite from the other three members of the group.

Cell dimensions were first determined on precession photographs taken with Zr-filtered Mo $K\alpha$ radiation. They were refined by least squares (Table 2) on 14 high-order reflections collected at 21°C on a 4-circle automated diffractometer with graphite-monochromated Ag $K\alpha$ radiation ($\lambda = 0.5609$Å). Systematic extinctions of $hkil$ reflections with $-h+k+l \neq 3n$ show mcGillite to be rhombohedral. Its Laue class is observed to be $\bar{3}2/m$ so that two space groups are possible, namely, $R3m$ or $R\bar{3}m$. A pyroelectric test proved negative, permitting us to assume space $R\bar{3}m$, at least provisionally.

Cell dimensions obtained by least-squares refinement of a powder pattern (Table 3) taken with Mn-filtered Fe $K\alpha$ radiation ($\lambda = 1.9373$ Å) also show satisfactorily low standard deviations, but differ appreciably from the values obtained on a single-crystal fragment from the same hand specimen (Table 2). Indeed the

TABLE 2. CRYSTAL DATA OF McGILLITE AND RELATED MINERALS

	Space group	a (Å)	c (Å)	Z	V/Z (Å^3)	Dm (g/cm^3)	Dx (g/cm^3)	n(ω)	n(ε)
McGillite	$R\bar{3}m$	13.498(3)* 13.459(9)	85.657(15)* 85.97(8)	24 24	563.1* 562.0	2.98(4) at 21°C	3.071	1.6685(15) NaD, 21°C	1.6415(15) NaD, 21°C
Friedelite	†R	13.40	21.43	6	555	3.041	3.060	1.654	1.625
Schallerite	$P\bar{3}m1$	13.43	14.31	4	559	3.339	3.338	1.704	1.679
Mangan-pyrosmalite	$P\bar{3}m1$	13.36	7.16	2	553	3.13	3.148	1.669	1.631
Pyrosmalite	$P\bar{3}m1$	13.35	7.15	2	552	3.153	3.101	1.675	1.636

McGillite: $(Mn_{6.95}Fe^{2+}_{0.63}Mg_{0.42})_{\Sigma=8.00}(Si_{5.94}Fe^{3+}_{0.06})_{\Sigma=6}[O_{14.94}(OH)_{8.21}Cl_{1.85}]_{\Sigma=25}$

Friedelite: $(Mn_{7.03}\square_{0.26}Mg_{0.25}Fe^{2+}_{0.21}Zn_{0.13}Ca_{0.12})Si_6[O_{14.00}(OH)_{10.47}Cl_{1.01}]$

Schallerite: $(Mn_{7.06}Mg_{0.61}Fe^{2+}_{0.19}Zn_{0.07}Ca_{0.07})(Si_{5.86}Fe^{3+}_{0.14})As^{3+}_{1.39}[O_{17.92}(OH)_{8.14}Cl_{0.03}]$

Mangan-pyrosmalite: $(Mn_{5.81}Fe^{2+}_{1.82}Zn_{0.25}Mg_{0.19})(Si_{5.99}As^{5+}_{0.01})[O_{14.725}(OH)_{9.57}Cl_{1.13}]$

Pyrosmalite: $(Fe^{2+}_{3.98}Mn_{3.53}Mg_{0.28}Ca_{0.08})(Si_{5.95}Al_{0.05})[O_{14.49}(OH)_{9.50}Cl_{1.21}]$

References: McGILLITE, present work; friedelite & schallerite, Bauer & Berman (1928); pyrosmalite and manganpyrosmalite, Frondel & Bauer (1953); optics of pyrosmalite from E.S. Larsen, in Bauer & Berman (1928). † Y. Takéuchi (1979; priv. comm.) reports $R\bar{3}m$. *Single-crystal data.

TABLE 3. COMPARISON OF McGILLITE AND FRIEDELITE POWDER PATTERNS

McGILLITE a=13.459(9), c=85.97(8)Å; R$\bar{3}$m				FRIEDELITE a=13.40, c=21.43Å; R$\bar{3}$m			
hk.ℓ	d_{calc}	d_{obs}	I	hk.ℓ	d_{calc}	d_{obs}	I
10. 1	11.55	11.67	2	10. 1	10.2	11.4	1
00.12	7.16	7.16	7	00. 3	7.17	7.17	9
11. 0	6.73	6.75	1	11. 0	6.70	-	-
$\bar{1}$0.11	6.49	6.50	1		-	-	-
$\bar{1}$0.14	5.43	5.44	1		-	-	-
00.24	3.582	3.570	4	00. 6	3.57	3.60	2
40. 4	2.888	2.888	6	40. 1	2.875	2.88	6
40.16	2.562	2.560	10	40. 4	2.55_1	2.56	10
$\bar{4}$0.20	2.412	2.409	2	$\bar{4}$0. 5	2.40_8	2.408	3
00.36	2.388			00. 0	2.38_1		
40.28	2.114	2.112	4	40. 7	2.10_8	2.115	4
10.40	2.114			10.10	2.10_7		
$\bar{4}$0.32	1.975	1.971	2	$\bar{4}$0. 8	1.968	1.974	2
11.48	1.731	1.727	2	11.12	1.725	1.731	3
40.40	1.730			40.10	1.724		
44. 0	1.682	1.683	4	44. 0	1.675	1.676	6
44.12	1.638	1.638	2	44. 3	1.631	1.632	2
$\bar{4}$0.44	1.623	1.619	2	$\bar{4}$0.11	1.617	1.625	1
44.24	1.523	1.524	1	44. 6	1.517	1.520	1
$\bar{8}$0. 4	1.454	1.454	1	$\bar{8}$0. 1	1.447	1.449	1
40.52	1.438	-	-	40.13	1.433	1.439	1
00.60	1.433	1.420	2	00.15	1.429	1.402	
11.60	1.401	-	-	11.15	1.397		
44.36	1.375	-	-	44. 9	1.370	1.374	1
$\bar{4}$0.56	1.358	1.356	2	$\bar{4}$0.14	1.354	1.359	3
$\bar{8}$0.28	1.316	1.317	1	$\bar{8}$0. 7	1.311	1.313	1
52.48	1.292	1.292	1	-	-	-	-
$\bar{8}$0.40	1.206	1.205	1	$\bar{8}$0.10	1.201	1.204	2
32.64	1.200	-	-	32.16	1.196	1.200	1
80.44	1.168	1.167	1	80.11	1.163	1.167	1
84. 4	1.100	1.100	1	84. 1	1.095	1.093	1
44.60	1.0908	1.0897	1	44.15	1.087	1.090	1
84.16	1.0789	1.0795	2	84. 4	1.074	1.065	1

McGILLITE pattern taken in a Debye-Scherrer camera with FeKα(Mn) radiation (λ=1.9373 Å) at 30 kV, 20 mA. 24.00hr. Cell dimensions from least-squares refinement of powder data. Estimated standard deviation shown between parentheses. FRIEDELITE data, d(obs) and I, from pattern (Frondel & Bauer 1953; Table 5) also taken with FeKα(Mn) radiation; space group by Y. Takéuchi (1979; priv. comm.).

difference between the two *c* lengths equals about four times the standard deviation of the less precisely determined powder value. The cell volume, however, remains constant to 0.2% from powder to single-crystal specimen, so that we are observing a change in cell shape, not in cell size.

The density of mcGillite, determined with the Berman balance on four cleavage fragments weighing between 15 and 25 mg, was found to be $D_m = 2.98(4)$ g/cm^3 at 21°C as compared with $D_x = 3.071$ g/cm^3 for 24 formula units *per* triple cell (hexagonal description). It is indistinguishable from the literature values for friedelite, but slightly lower than the densities given for schallerite, manganpyrosmalite and pyrosmalite (Table 2). Cleavage is easy and good in one direction {0001}, difficult but fair in three directions {10$\bar{1}$1}. The Vickers hardness ranges from 278 to 330 kg/mm^2 measured with a load of 15 grams.

McGillite is light to dark pink in color, with pearly lustre on its basal cleavage. Refractive indices n_ω and n_ϵ of mcGillite are also in the range covered by the other four members of the pyrosmalite group (Table 2). They were measured by oil immersion, in sodium light, at 21°C. Occasional fragments show biaxial (–) character up to $2V \sim 10°$, but even these show perfect rhombohedral symmetry on single-crystal X-ray patterns.

A Gladstone–Dale *K* value of 0.223 is derived from the composition (Table 1) and the constants of Mandarino (1976). It compares reasonably well with the value of 0.215 obtained from the average refractive index and the calculated density, D_x (Table 2). Throughout the mineralogical literature *K* has been called the "specific refractive energy" (of a given compound). Let us note, however, that *K* is *not* an energy term since its definition, $K = n{-}1/d$, makes it a dimensionless constant or gives it dimensions of volume/mass depending on whether *d* stands for specific gravity or density. The better term *specific refractivity* is used by physicists (Gray 1972, p. 6-8).

The powder patterns of mcGillite and friedelite are extremely similar, which is not surprising since the Mn^{2+} atoms, much the heaviest atoms in the crystal structure, form the same substructure in the two mineral species. Powder-line intensities were calculated by F.L. Lee from the manganese coordinates of the friedelite structure (Kashaev & Drits 1973) and by V.J. Donnay from a complete trial structure for which a special program was written, giving 2θ, *d*, *hk.l* and I_{calc}. These intensities are roughly in line with the observed values. Only three faint lines, $\bar{1}$0.11 at $d = 6.50(1)$, $\bar{1}$0.14 at $d = 5.44(1)$ and 52.48 at $d = 1.292(2)$ Å distinguish the mcGillite powder pattern from that of friedelite (Table 3).

We have found that a quick and reliable way to identify mcGillite crystallographically is to mount a fragment with a cleavage face (0001) in polar position, where it can be adjusted accurately on the 2-circle goniometer, and to take a *c*-rotation pattern (Fig. 1). The combination of the unusually short c^* repeat (c = 85.7 Å) and the pronounced diffuse streaks that outline the row lines parallel to c^* enables mcGillite to be readily identified. The diffuse streaks are also strikingly shown on a *c* cone-axis photograph (Fig. 2).

CRYSTAL-STRUCTURE CONSIDERATIONS

With appropriate modification, the atomic coordinates of the three-layer friedelite structure (Kashaev & Drits 1973) are being used as a

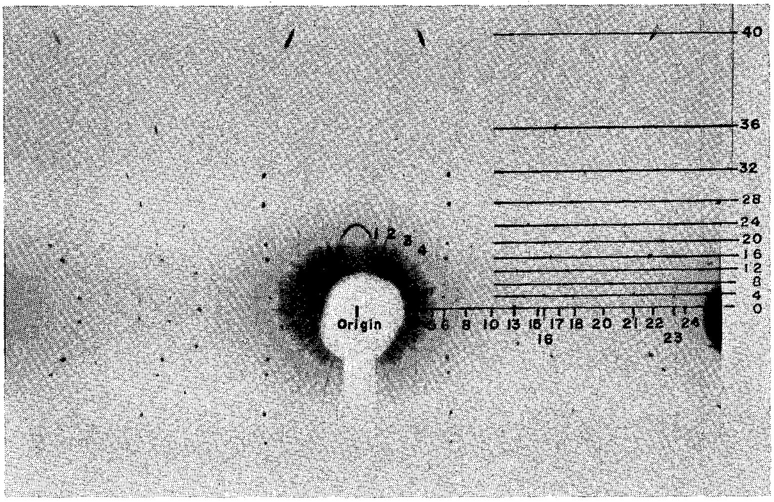

FIG. 1. McGillite rotation pattern about the *c* axis. Mn-filtered Fe K_α, 30 kV, 14 mA, 30 h. Layer lines with *l* a multiple of 4 are shown on the right, with values from 0 to 40. The row lines, numbered from 1 through 24, have their *h* and *k* values identified from 1 to 16 as follows: 1: 2,0; 2: 2,1; 3: 2,2; 4: 4,0; 5: 4,1; 6: 5,0; 7: 4,3; 8: 5,2; 9: 4,4; 10: 6,2; 11: 7,1; 12: 5,4; 13: 8,0; 14: 8,1; 15: 9,0; 16: 8,4.

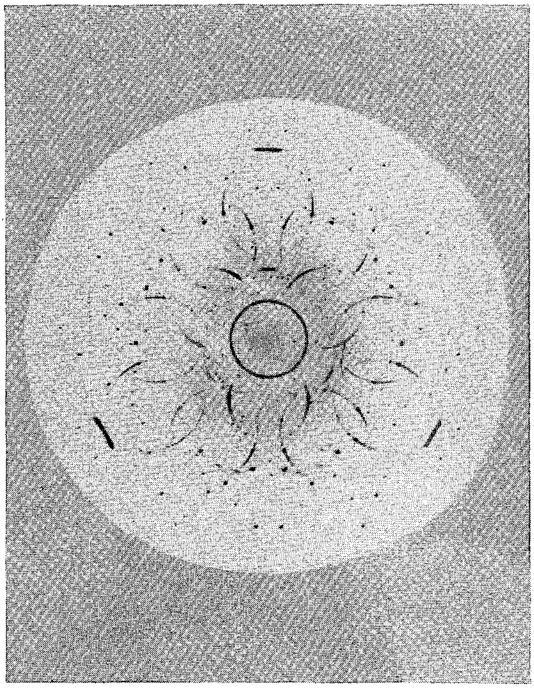

FIG. 2. McGillite *c*-cone-axis precession photograph; $\mu = 10°$, s = 40.0 mm. Zr-filtered Mo K_α, 40kV, 20mA, 40 h. The intense, diffuse rods parallel to c^* transform the usual design of concentric circles into a "fingerprint" unique to mcGillite.

starting point for the structure determination of the twelve-layer mcGillite structure. In each layer, a brucite-type $\mathrm{Mn(OH,Cl,O)}_{z=2}$ sheet shares its oxygen atoms with neighboring silicate sheets of the zeolitic type first assigned to this mineral group by Takéuchi *et al.* (1963). The combination of Mn and Si sheets into one, or more than one, layer leads to space group $P\bar{3}m1$ in one-layer pyrosmalite and manganpyrosmalite and in two-layer schallerite, but its description requires $R\bar{3}m$ for the friedelite and mcGillite structures. In all five minerals, the manganese substructure quarters both *a* and *c*, within the experimental accuracy with which the manganese coordinates have been determined, thus explaining the fact that the strong powder lines have all their indices multiples of four (Table 3). Beginning with the Mn sheet at $z = 0$, one Mn atom is placed at the origin, 0,0,0; in the adjacent sheet at $z = 1/12$ the corresponding Mn atom is moved to 11/12, 1/12, 1/12, *etc.*

The silicate sheets, consisting of 12-, 6- and 4-membered rings of SiO_4 tetrahedra of point symmetries $\bar{3}m$, $3m$ and $\bar{1}$ respectively, suffer considerable distortion in the process of fitting the apical oxygen atoms of their tetrahedra into the two adjacent Mn sheets. The chlorine atoms fit randomly into 54 sites, as mentioned above.

The rods of continuous, diffuse intensity parallel to c* in weighted reciprocal space are due to disorder in the stacking of silicate sheets. The major obstacle encountered in the structure refinement of mcGillite is the limited number of observable 3-dimensional reflections with $h, k, l \neq 4n$. The indexed rotation-pattern (Fig. 1) illustrates this dilemma. We are therefore continuing our search for an exceptionally well-ordered single crystal of mcGillite that will yield more of the faint Bragg reflections for inclusion in Fourier syntheses and least-squares refinement of positional and thermal parameters and chemical occupancies.

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SUGILITE, A SECOND OCCURRENCE: WESSELS MINE, KALAHARI MANGANESE FIELD, REPUBLIC OF SOUTH AFRICA

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ABSTRACT

Sugilite, a sodium potassium ferric iron silicate, has been found in the Wessels mine, Kuruman district, Northern Cape Province, Republic of South Africa. It occurs as violet seams in manganese ore. It bears no visual resemblance to the type material. Microprobe analysis yields 69.6 SiO_2, 13.9 Fe_2O_3, 1.9 MnO, 4.7 K_2O and 6.0 Na_2O, total 96.1, by weight. The mineral is abundant and is associated with acmite and braunite in sedimentary beds.

Keywords: sugilite, alkali iron silicate, Wessels mine, Republic of South Africa, manganese ore, Kalahari.

SOMMAIRE

On a trouvé la sugilite, silicate de sodium, potassium et fer ferrique, dans la mine Wessels, district de Kuruman, dans le Nord de la province du Cap, république de l'Afrique du Sud. En veinules violacées dans un minerai de manganèse, cette sugilite ne ressemble aucunement à son type. Une analyse à la microsonde donne 69.6 SiO_2, 13.9 Fe_2O_3, 1.9 MnO, 4.7 K_2O et 6.0 Na_2O, total 96.1 (en poids). La sugilite se trouve ici en abondance, associée à l'acmite et à la braunite dans des couches sédimentaires.

(Traduit par la Rédaction)

Mots-clés: sugilite, silicate alcalin de fer, mine Wessels, république de l'Afrique du Sud, minerai manganésifère, Kalahari.

INTRODUCTION

Sugilite was originally described from the northeastern part of Iwagi Islet, Ehime Prefecture, Japan, by Murakami *et al.* (1976). There it occurs as isolated grains in an acmite syenite stock emplaced in biotite granite. Sugilite is associated with albite, acmite, pectolite, allanite, titanite, zircon and andradite.

This second occurrence of sugilite was originally called to the attention of the senior author by Dr. Robert Gait and Mr. Prosper Williams of Toronto. Additional samples from the same locality came to us through various individuals, to whom we are deeply indebted. This sugilite occurs at the Wessels mine, 22.5 km northwest of Hotazel in the Kuruman district, Cape Province, Republic of South Africa. The mine, owned and operated by S. A. Manganese Armcor Ltd. of Johannesburg, was opened in May, 1973. The ore bodies generally are layered, with different groups of minerals predominating in different layers. The minerals are always intimately intergrown and difficult to identify by macroscopic methods. Discussions of the geology of the surrounding Kalahari manganese field have been adequately presented by de Villiers (1967), Coetzee (1976) and Wilson & Dunn (1978). According to Dr. P. R. de Villiers (pers. comm. 1977), the sugilite was found by accident in 1973 when the roof of an inclined shaft caved in during development. Apparently no other occurrences were found, and we have no further information on this one.

DESCRIPTION

In the Wessels mine, sugilite occurs as bedded

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seams (up to 3 cm thick) of massive material interlayered with fine-grained acmite and various manganese oxides, chiefly braunite. The color of this sugilite is very dark to light violet; the color darkens with increasing abundance of acmite inclusions. The acmite can appear almost opaque with vitreous lustre and a quartzite-like texture where heavily saturated with braunite inclusions. The sugilite has a vitreous lustre with a granular texture. No single crystals were found; the mineral occurs only in a massive fine-grained state. The Mohs hardness of the Wessels-mine sugilite is 5½ to 6, slightly softer than the 6–6½ value reported for the type material from Japan. The density, determined with heavy-liquid techniques, is 2.79 g/cm^3, in good agreement with the theoretical value of 2.80 g/cm^3 calculated for the type material, which has similar composition. Optically, sugilite is uniaxial negative with refractive indices ω 1.611(3) and ϵ 1.605(3). It is very weakly pleochroic and does not respond to ultraviolet radiation.

The X-ray powder-diffraction pattern of this sugilite is identical to that of the type material from Japan. There are no discernible differences in the diffraction patterns obtained with a 114.6 mm diameter Gandolfi camera, a multicrystalline ball-mount and Cu $K\alpha$ X radiation.

We note with interest that a description of what seems to be the same mineral has been published as sogdianite by Bank *et al.* (1978). The X-ray powder patterns of sogdianite and sugilite are nearly identical, considering the strongest lines. We note the absence of zirconium in our material and suggest the possibility that the phases could have been confused.

CHEMICAL COMPOSITION

The sugilite described here was chemically analyzed with an ARL–SEMQ electron microprobe using an operating voltage of 15 kV and a beam current of 0.15 μA. The standards used were manganite for manganese, hornblende for calcium, iron, magnesium, sodium and potassium, and zektzerite for silicon. The data were corrected using Bence–Albee factors. An emission-spectrograph analysis confirmed the microprobe results and, in addition, indicated the presence of lithium in the 1–10% range, by weight. The resultant microprobe analysis is compared with the analysis of Murakami *et al.* (1976) in Table 1.

TABLE 1. CHEMICAL DATA FOR SUGILITE

	Wessels mine	Japan
SiO_2	69.6	71.38
TiO_2	0.0	0.51
Al_2O_3	0.0	2.97
Fe_2O_3	13.9*	12.76
FeO	n.d.	0.19
MgO	0.0	n.g.
CaO	0.0	0.0
MnO	1.9	n.g.
K_2O	4.7	3.76
Na_2O	6.0	4.37
Li_2O	**	3.14
H_2O^+	0.0***	0.81
H_2O^-	0.0	0.12
Total	96.1	100.01

Accuracy of data on sugilite from Wessels mine: 3% of amount present. * Iron determined as total iron and calculated as Fe^{3+} based on known state of Fe in sugilite. ** Lithium present as a major element. *** H_2O determined by DTA/TGA. NMNH sample # 137289.

Manganese is not a major component in this sugilite. Although the material has been sold under the name of *manganese analogue of sugilite,* it is a "normal" sugilite with but minor replacement of iron by manganese. Owing to the complexities of the osumilite group, to which sugilite probably belongs, we cannot directly ascribe the available manganese to a specific valence state; therefore, we calculate it here as MnO simply for convenience. Lithium is present in significant amounts. However, this sugilite is thoroughly intergrown with microscopic crystals of acmite with a composition very near the end member and containing about 0.8% MnO. The abundant inclusions in the sugilite rendered useless an attempt to determine lithium quantitatively by flame-photometry methods and wet chemistry. However, the presence of abundant lithium was proven by ion-microprobe mass spectroscopy and further confirms the identity of this material as sugilite. DTA/TGA analysis indicates that the material has less than 0.02% H_2O and melts at approximately 895°C to a pale brown glass. The analysis refers to the darkest violet material.

The sugilite from Japan contains 3.14% Li_2O. If we calculate lithium by difference, we obtain 3.9% Li_2O for the Wessels-mine sugilite. However, if we were to use this calculated figure, the estimated error of the microprobe analysis (± 3% of the amount present) would greatly affect the number of lithium atoms in the unit cell. Hence, we cannot calculate the number of cations *per* unit cell with reliability. Given the extensive substitutions possible in the osumilite group and the undetermined oxidation state of the iron, we cannot assign the cations to specific sites without a crystal-structure determination.

CONCLUSIONS

In summary, sugilite from the Wessels mine is distinctly different from the type material in physical appearance. The mineral is no longer a rare species; it was found in kilogram quantities and in 1977 was noted in South Africa by Mr. Prosper Williams, being used for ashtrays.

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