



Article

Discreditation of the pyroxenoid mineral name ‘marshallsussmanite’ with a reinstatement of the name schizolite, $\text{NaCaMnSi}_3\text{O}_8(\text{OH})$

Joel D. Grice^{1*}, Aaron J. Lussier¹, Henrik Friis², Ralph Rowe¹, Glenn G. Poirier¹ and Zina Fihl³

¹Canadian Museum of Nature, PO Box 3443 Stn D, Ottawa Canada, K1P 6P4, Canada; ²Natural History Museum, University of Oslo, PO Box 1172, Blindern, 0318 Oslo, Norway; and ³Natural History Museum of Denmark, Øster Volgade 5-7, 1350 Copenhagen K, Denmark

Abstract

Schizolite, originating from the type locality, Tutop Agtakórfia, in the Ilímaussaq alkaline complex, Julianehåb district, South Greenland, was described initially by Winther (1901) with additional data being supplied by Bøggild (1903). Recently, a proposal for the new mineral ‘marshallsussmanite’ was submitted to, and approved by, the International Mineralogical Association Commission on New Minerals, Nomenclature and Classification (IMA2013-067) by Origlieri *et al.* (2013). Results from the detailed examination of two schizolite cotype samples presented here, using single-crystal and powder X-ray diffraction, and optical properties, confirms it to be equivalent to ‘marshallsussmanite’. Historical precedence sets a priority for discrediting the name ‘marshallsussmanite’ in favour of the original, more-than-a century-old name, schizolite. The two schizolite samples investigated vary slightly in physical and chemical properties but are consistent overall. The prismatic crystals are pale red or pink to brownish. Schizolite is brittle with a splintery aspect. It is biaxial (+), with average optical parameters: $\alpha = 1.626 \pm 0.003$, $\beta = 1.630 \pm 0.002$, $\gamma = 1.661 \pm 0.002$, $2V_{\text{meas}} = 71(4)^\circ$ and $2V_{\text{calc}} = 40^\circ$; there is no pleochroism. Electron microprobe analysis shows both samples have nearly identical compositions (differences <0.4 wt.% oxide), with the mean values of: SiO_2 52.6(4); Al_2O_3 0.005(1); FeO 2.54(2); MnO 13.86(9); CaO 17.9(4); Na_2O 8.9(1); and H_2O 2.59(2) wt.% oxide; this corresponds to a mean formula of: $\text{Na}_{1.00(2)}\text{Ca}_{1.11(7)}\text{Mn}_{0.68(1)}\text{Fe}_{0.12(0)}\text{Si}_{3.041(1)}\text{O}_8(\text{OH})$. Final least-squares structure refinements for both samples converged at R_1 values $\leq 2.0\%$; H atoms were located in all refinements.

(Received 10 December 2018; accepted 10 March 2019; Accepted Manuscript online: 22 April 2019; Associate Editor: Ferdinando Bosi)

Introduction

The new mineral proposal for ‘marshallsussmanite’ (IMA2013-067) was approved in October 2013 and the abstract was published in the *Mineralogical Magazine* (Origlieri *et al.*, 2013). In the proposal, the authors made no comparison between ‘marshallsussmanite’ and schizolite yet they knew schizolite existed as they referred to the crystal structure reported by Ohashi and Finger (1978). The crystal structure of ‘marshallsussmanite’ has not been officially published, but it is recorded in IMA proposal and can be found as a ‘preproof’ on the *Mineralogical Magazine* website (Origlieri *et al.*, 2017). Since then, Nagashima *et al.* (2018) refined the structure of a ‘marshallsussmanite’.

In this brief account, we have re-characterised the cotype material from Tutop Agtakórfia, Greenland in order to show that ‘marshallsussmanite’ and schizolite are the same mineral species. This validates the authenticity of schizolite and re-establishes the type material. For historical reasons the name schizolite must be given priority. The discreditation of ‘marshallsussmanite’, with a reinstatement of the name schizolite, has been proposed and it has been approved by the IMA-CNMNC (Voting proposal 18-B,

February 19, 2018, Hålenius *et al.*, 2018). Two samples of schizolite are examined here in detail (labelled NHMD 1899.856 and NHMD 1899.8), both originating from the original type locality.

History of schizolite characterisation

The type locality of schizolite is Tutop Agtakórfia (Petersen and Johnsen, 2005), in the Ilímaussaq alkaline complex, Julianehåb district, South Greenland. The type material is stored in the Geological Museum, now a part of the Natural History Museum of Denmark. In 1901 schizolite was described as a new mineral species by Winther based on material collected by Flink in 1897: “*The new mineral, on account of its properties, is allied to the pectolite group.*” He goes on to say: “*Both in composition and crystallographic properties the schizolite differs distinctly from pectolite, so it is undoubtedly correct to classify it as a special mineral.*” Winther (1901) named the mineral schizolite based on its ‘schizo’ or ‘split’ cleavage. Shortly afterwards, Bøggild (1903) reported that the mineral is triclinic and not monoclinic, working on material that he himself had collected at the type locality in 1899.

These first studies of schizolite from Ilímaussaq showed a difference in appearance and composition, with the Tutop Agtakórfia material typically being pinker than material from the other localities where the colour is often more grey-to-brownish (Flink, 1898; Winther, 1901; Bøggild, 1903). Bøggild

*Author for correspondence: Joel D. Grice, Email: jgrice@nature.ca

Cite this article: Grice J.D., Lussier A.J., Friis H., Rowe R., Poirier G.G. and Fihl Z. (2019) Discreditation of the pyroxenoid mineral name ‘marshallsussmanite’ with a reinstatement of the name schizolite, $\text{NaCaMnSi}_3\text{O}_8(\text{OH})$. *Mineralogical Magazine* 83, 473–478. <https://doi.org/10.1180/mgm.2019.21>



Fig. 1. (a) Schizolite collected by Gustaf Flink in 1897 and used in the original description by Christian Winther (1901); catalogue NHMD 1899.856. (b) Schizolite collected by Ove Balthasar Bøggild and Brunnurstedt in NHMD 1899; catalogue NHMD 1899.8

(1903) compared the composition of schizolite from different localities within Ilímaussaq and found that the pink material has higher Mn^{2+} content than the other coloured schizolite, even when the two types occur at the same locality.

Schaller (1955) effectively discredited this species as a manganoan pectolite, stating that “*The term schizolite can be discarded as an unnecessary species name.*” The simplest formula was established as $Na(Ca,Mn)_2Si_3O_8(OH)$. In this study, there was only powder diffraction data and chemical analysis, no crystal-structure analysis, and the differentiation of species in the series was not possible at this time without the structure. Further, this was done prior to the establishment of the Commission of New Minerals, Names and Classification, International Mineralogical Association (IMA-CNMNC) in 1959 and cannot be considered as an official discreditation.

Ohashi and Finger (1978) established the validity of the schizolite species with a crystal-structure analysis that defined the ordering of the cations Ca and Mn^{2+} between the two octahedrally-coordinated sites, $M1$ and $M2$, making a distinction between the three isostructural species; pectolite ($Na^{M1}Ca^{M2}CaSi_3O_9H$), schizolite ($Na^{M1}Ca^{M2}MnSi_3O_9H$) and serandite ($Na^{M1}Mn^{M2}MnSi_3O_9H$). However, these authors did not emphasise that this made schizolite a different species. In fact, Petersen and Johnsen (2005) list schizolite as a doubtful species, but this can now be rectified.

Table 1. Comparison of schizolite, ‘marshallsussmanite’, serandite and pectolite.

Mineral species (data reference)	Serandite	Schizolite	‘Marshallsussmanite’	Schizolite	Schizolite	Pectolite
Formula (ideal)	$NaMnMnSi_3O_8(OH)$	$NaCaMnSi_3O_8(OH)$	$NaCaMnSi_3O_8(OH)$	(NHMD 1899.856) $NaCaMnSi_3O_8(OH)$	(NHMD 1899.8) $NaCaMnSi_3O_8(OH)$	$NaCaCaSi_3O_8(OH)$
Formula (empirical)	$Na_{0.88}Mn_{1.47}Ca_{0.67}Si_{2.93}O_9H_{1.06}$	$Na_{1.07}Ca_{1.21}Mn_{0.63}Fe_{0.14}Si_{2.93}O_9H_{0.53}$	$Na_{0.93}Ca_{0.96}Mn_{1.07}Si_{3.01}O_9H$ ($Na_{0.948}Ca_{1.052}$) $M1(Ca_{0.793}Mn_{0.207})$ $M2(Ca_{0.937}Mn_{0.063})$	$Na_{0.93}Ca_{0.917}Mn_{1.08}Si_{3.01}O_9H$ $Na^{M1}(Ca_{0.734}Mn_{0.266})$ $M2(Mn_{0.817}Ca_{0.183})$	$Na^{M1}(Ca_{0.772}Mn_{0.228})$ $M2(Mn_{0.813}Ca_{0.187})$	$Na_{0.97}Ca_{1.98}Si_{2.97}O_9H_{1.20}$
Formulae (SREF)	—	—	$Si_3O_8(OH)$	$Si_3O_8(OH)$	$Si_3O_8(OH)$	—
Physical properties	Bladed, salmon-red ^a ; peach ^b	Prismatic, pink to brown ^b	Bladed, orange-tinted pink	Pale pink	Pale brown	Prismatic, colourless to white ^{a,b}
Density (g cm ⁻³)	3.34 ^a	3.05 ^a	3.17	3.17	2.90 ^a	2.90 ^a
Optical properties	1.668, 1.671, 1.703	1.631, 1.636, 1.660	1.641, 1.646, 1.671	1.626(3), 1.630(2), 1.661(2)	1.640(3), 1.643(2), 1.658(2)	1.610, 1.615, 1.643
α , β , γ (°)	39 ^a	47 ^a	49	72(4)	52(2)	53 ^a
2V (°)	P _I	P _I	P _I	P _I	P _I	P _I
Space group	—	—	—	—	—	—
Cell parameters	7.719, 6.906, 6.762	7.868, 6.978, 6.920	7.783, 6.937, 6.850	7.855(2), 6.9715(2), 6.9173(2)	7.8492(1), 6.9752(1), 6.9117(1)	7.988, 7.040, 7.025
a , b , c (Å)	90.50, 94.09, 102.78	90.72, 94.53, 102.92	90.68, 94.33, 102.85	90.756(1), 94.489(1), 102.858(1)	90.791(1), 94.452(1), 102.849(1)	90.52, 95.18, 102.47
α , β , γ (°)	350.6 ^b	366.4 ^b	359.4	367.99(1)	367.64(1)	384.0 ^b
Sample locality	Rouma Isle, Guinea ^a ; Mont Saint-Hilaire, Canada ^b	Kangerdluarssuk, Greenland	Wessels mine, South Africa	Tutup, Agtakórfia, Greenland	Tutup, Agtakórfia, Greenland	Lovozero, Russia ^a ; Bergen Hill, New Jersey ^b
References	A. Lacroix (1931) B. Jacobsen et al. (2000)	A. Schaller (1955) B. Ohashi and Finger (1978)	Origlieri et al. (2013)	This study	This study	A. Schaller (1955) B. Prewitt (1967)

Table 2. Chemical analyses: schizolite and pectolite from Tutop Agtakórfia.

Sample no.	NHMD 1899.856 ¹ Schizolite (cotype) 26 analyses		NHMD 1899.8 ² Schizolite (cotype) 21 analyses	
	Average Wt.%	Range	Average Wt.%	Range
SiO ₂	52.17(24)	51.33–52.51	52.95(52)	51.80–54.36
Al ₂ O ₃	0.06(12)	0.03–0.66	0.04(1)	0.02–0.06
FeO	2.52(16)	2.20–2.80	2.56(15)	2.26–2.91
MnO	13.95(50)	12.81–14.77	13.77(94)	12.39–15.80
MgO	0.00(1)	0.00–0.01	0.02(6)	0.00–0.26
CaO	17.49(48)	16.69–18.61	18.27(82)	17.19–20.18
Na ₂ O	9.01(17)	8.23–9.19	8.84(16)	8.46–9.11
H ₂ *	2.57(1)	2.25–2.59	2.61(2)	2.57–2.66
Total	97.77(53)	95.50–98.58	99.06(91)	97.54–100.68

¹Na_{1.02}Ca_{1.09}Mn_{0.69}Fe_{0.12}Si_{3.04}H₁O₉; ²Na_{0.98}Ca_{1.12}Mn_{0.67}Fe_{0.12}Si_{3.04}H₁O₉; atomic fractions calculated of the basis of 9 oxygen atoms.

*H₂O calculated on the basis of 1 H apfu

Study material

Two samples of cotype material are investigated here, both originating from the type locality: (1) *Sample NHMD 1899.856*: This material was studied by Winther (1901) after being collected by Gustaf Flink in 1897 (Fig. 1a). This specimen is part of a suite of 14 specimens studied by Winther, with an additional seven that were also probably part of his research. Winther named the new mineral schizolite, and as this is the first description of the

mineral, it is undoubtedly the type material. (2) *Sample NHMD 1899.8*: This material was collected by Bøggild and Brunnurstedt, in 1899 and studied in greater detail by Bøggild (1903) (Fig. 1b). It is part of a suite of 11 specimens. Both specimens were graciously provided by the Natural History Museum of Denmark in Copenhagen. All material used for optical measurements, crystal structure analysis and microprobe data collections has been returned; none has been retained at the Canadian Museum of Nature.

Methods and results

Physical and optical properties

At the type locality, schizolite occurs as stacked prismatic columns, up to 2 cm long. These occur as either individual crystals or aggregates of crystals. The mineral is pale pink to brownish with a white streak and vitreous lustre. It is translucent to opaque, non-fluorescent and has a hardness (Mohs) \approx 5. The mineral is brittle with two perfect cleavages making it splintery or somewhat fibrous. The calculated density is 3.09 g cm⁻³.

Pale pink schizolite (NHMD 1899.856) is biaxial (+) with $\alpha = 1.626 \pm 0.003$, $\beta = 1.630 \pm 0.002$, $\gamma = 1.661 \pm 0.002$, $2V_{\text{meas}} = 72(4)^\circ$ and $2V_{\text{calc}} = 40^\circ$. Pale brown schizolite (NHMD 1899.8) is biaxial (+) with $\alpha = 1.640 \pm 0.003$, $\beta = 1.643 \pm 0.002$, $\gamma = 1.658 \pm 0.002$, $2V_{\text{meas}} = 52(2)^\circ$, $2V_{\text{calc}} = 49^\circ$. There is no pleochroism observed in either specimen. Optical parameters were measured on a crystal

Table 3. Powder X-ray diffraction data for schizolite ($K\alpha_1$) (sample# NHMD 1899.856)

<i>l</i> _{obs.}	<i>l</i> _{calc.} *	<i>d</i> _{obs.}	<i>d</i> _{calc.} *	<i>h k l</i>	<i>l</i> _{obs.}	<i>l</i> _{calc.} *	<i>d</i> _{obs.}	<i>d</i> _{calc.} *	<i>h k l</i>	<i>l</i> _{obs.}	<i>l</i> _{calc.} *	<i>d</i> _{obs.}	<i>d</i> _{calc.} *	<i>h k l</i>
12	15	7.624	7.6261	1 0 0	3	2	2.455	2.4561	0 $\bar{2}$ 2	3	4	1.7572	1.7629	2 $\bar{2}$ 3
11	14	6.884	6.8866	0 0 1	3	3	2.455	2.4555	2 0 2	4	4	1.7579	1.7579	4 2 1
	5		6.7940	0 1 0	9	2	2.412	2.4275	$\bar{1}$ 2 2	4	3	1.7496	1.7496	3 2 1
4	5	5.338	5.3378	$\bar{1}$ 0 1	19	19	2.4113	2.4113	1 $\bar{2}$ 2	3	3	1.7451	1.7451	1 2 3
2	2	4.908	4.9121	0 $\bar{1}$ 1	8	15	2.381	2.3821	0 2 2	10	28	1.7431	1.7431	1 $\bar{4}$ 0
4	7	4.590	4.5868	1 1 0	15	14	2.296	2.2980	3 $\bar{2}$ 0	3	3	1.7369	1.7369	4 1 0
3	6	4.499	4.4995	$\bar{1}$ 1 1	6	6	2.2955	2.2955	0 0 3	7	13	1.7215	1.7217	0 0 4
2	4	4.339	4.3377	1 $\bar{1}$ 1	8	8	2.2934	2.2934	2 $\bar{2}$ 0	8	6	1.6829	1.6832	$\bar{2}$ $\bar{2}$ 3
5	9	3.951	3.9489	$\bar{1}$ $\bar{1}$ 1	3	3	2.2707	2.2707	1 $\bar{2}$ 2	13	13	1.6820	1.6820	$\bar{3}$ $\bar{2}$ 2
13	18	3.813	3.8131	2 0 0	19	27	2.251	2.2507	$\bar{1}$ 0 3	6	15	1.6749	1.6748	4 2 2
3	2	3.700	3.6987	2 $\bar{1}$ 0	3	3	2.2497	2.2497	$\bar{2}$ 2 2	3	5	1.6702	1.6705	$\bar{3}$ 2 3
9	13	3.443	3.4433	0 0 2	3	5	2.221	2.2226	3 1 0	2	5	1.6367	1.6370	3 0 3
3	2	3.394	3.4000	1 $\bar{2}$ 0	4	3	2.196	2.1954	2 1 2	2	4	1.6215	1.6208	$\bar{2}$ 0 4
	3		3.3970	0 2 0	2	2	2.1952	2.1952	0 $\bar{1}$ 3	2	7	1.5876	1.5872	4 2 2
4	4	3.348	3.3497	$\bar{2}$ 2 1	3	3	2.170	2.1685	$\bar{3}$ $\bar{1}$ 1	3	6	1.5775	1.5770	3 2 2
34	48	3.241	3.2415	$\bar{1}$ 0 2	8	14	2.146	2.1448	3 $\bar{2}$ 1	3	9	1.5418	1.5421	0 4 2
26	32	3.225	3.2236	2 0 1	12	7	2.132	2.1320	$\bar{3}$ 0 2	2	4	1.5266	1.5309	$\bar{4}$ 0 3
12	16	3.111	3.10999	0 $\bar{1}$ 2	16	16	2.1311	2.1311	2 2 1	4	4	1.5284	1.5284	$\bar{2}$ 4 2
	2		3.0456	2 1 0	4	3	1.9085	1.9085	$\bar{2}$ $\bar{1}$ 3	4	4	1.5254	1.5254	5 $\bar{2}$ 0
42	58	3.047	3.0443	1 0 2	2	2	1.9084	1.9084	$\bar{1}$ 2 3	2	3	1.5230	1.5229	4 2 0
50	16	3.044	3.0342	0 1 2	3	3	1.9065	1.9065	4 0 0	2	2	1.5166	1.5203	2 4 2
15	25	3.005	3.0045	$\bar{1}$ 1 2	2	2	1.8966	1.8966	1 $\bar{2}$ 3	2	2	1.5171	1.5171	0 2 4
4	9	2.910	2.908	1 $\bar{1}$ 2	2	2	1.8779	1.8782	$\bar{4}$ 0 1	2	2	1.5161	1.5161	5 0 1
100	93	2.875	2.8779	2 $\bar{2}$ 0	2	2	1.8756	1.8756	0 2 3	2	2	1.5155	1.5155	$\bar{1}$ 2 4
	100		2.8725	1 2 0	2	2	1.8664	1.8661	0 3 2	4	10	1.4638	1.4635	5 0 1
	4		2.8724	$\bar{2}$ $\bar{1}$ 1	2	2	1.8647	1.8647	3 $\bar{2}$ 2	5	12	1.4536	1.4535	2 2 4
	2		2.8525	$\bar{1}$ $\bar{1}$ 2	3	4	1.8504	1.8532	$\bar{2}$ 3 2	6	12	1.4406	1.4408	1 2 4
6	12	2.707	2.7068	$\bar{1}$ $\bar{2}$ 1	5	5	1.8492	1.8492	2 3 2	2	5	1.3731	1.3732	3 0 4
4	9	2.692	2.6912	$\bar{2}$ 2 1	3	4	1.8287	1.8280	$\bar{2}$ 2 3	4	3	1.3535	1.3534	$\bar{2}$ 4 2
12	23	2.670	2.6689	$\bar{2}$ 0 2	2	3	1.8204	1.8228	2 $\bar{3}$ 2	5	5	1.3533	1.3533	5 0 2
6	11	2.579	2.5786	3 $\bar{1}$ 0	2	2	1.8186	1.8186	$\bar{3}$ $\bar{2}$ 1					
14	26	2.543	2.5420	3 0 0	5	5	1.8009	1.8009	$\bar{1}$ 3 2					
					4	4	1.7992	1.7992	4 0 1					

*Calculated from structure data modified with Rietveld software.

Refined cell $a = 7.85062(14)$ $b = 6.97283(8)$ $c = 6.91131(11)$ Å, $\alpha = 90.695(2)$, $\beta = 94.5174(18)$, $\gamma = 102.8861(12)^\circ$, $V = 367.487(2)$ Å³

The strongest lines are given in bold

Table 4. Data and experimental details for schizolite, Tutop Aqtakórfia NHMD 1899.856 (cotype), Greenland.

Crystal data	
Ideal unit-cell contents	2[NaCaMnSi ₃ O ₉ H]
Crystal system, space group	Triclinic, $P\bar{1}$ (SG # 2)
Temperature (K)	293(2)
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.8551(2), 6.9715(2), 6.9173(2)
α , β , γ (°)	90.756(1), 94.489(1), 102.858(1)
<i>V</i> (Å ³)	367.99(1)
<i>Z</i>	2
Calculated density (g cm ⁻³)	3.09
μ (mm ⁻¹)	3.54
Data collection	
Instrument	Bruker APEX II
Radiation type, wavelength (Å)	MoK α , λ = 0.71073
θ range (°)	2.669–36.439
Absorption correction	Multi-scan (TWINABS-2012/1, Bruker, 2012)
No. of measured, independent and observed [$F > 4\sigma(F)$] reflections	17034, 3588, 3443
R_{int}	0.014
Indices range of <i>h</i> , <i>k</i> , <i>l</i>	–13 ≤ <i>h</i> ≤ 13, –11 ≤ <i>k</i> ≤ 11, –11 ≤ <i>l</i> ≤ 11
Refinement	
Refinement	full-matrix least squares on F^2
Number of reflections, parameters	3588, 141
Number l.s. parameters	150
$F(000)$	347.0
<i>R</i> index for all data	0.015
<i>R</i> index for observed data	0.014
wR^2 for all data	0.044
GoF on F^2	0.955
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e ⁻ Å ⁻³)	0.54, –0.30

$$R_1 = \sum ||F_{\text{obs}}| - |F_{\text{calc}}|| / \sum |F_{\text{obs}}|; wR_2 = \left[\frac{\sum [w(F_{\text{obs}}^2 - F_{\text{calc}}^2)^2]}{\sum w(F_{\text{obs}}^2)^2} \right]^{1/2}$$

$$\text{GoF} = \left[\frac{\sum [w(F_{\text{obs}}^2 - F_{\text{calc}}^2)^2]}{\sum w(F_{\text{obs}}^2)^2} \right]^{1/2} w = 1/[\delta^2(F_0^2) + (0.0269 \times P)^2 + 0.20 \times P] \text{ where } P = (\text{Max}(F_0^2, 0) + F_0^2) / 3$$

fragment using a spindle stage with Na light, $\lambda = 590$ nm, and the measured 2V was determined from extinction curves. It was particularly difficult to measure α in this mineral, as the observation direction is down a crystal fragment edge. Comparative optical properties for current and other members of the series are given in Table 1.

Chemical analysis

The chemical analyses were performed on a JEOL 8230 electron microprobe operating in wavelength-dispersion (WD) mode using *Probe for EPMA* software (<https://www.probesoftware.com>). The operating voltage was 20 kV, the beam current was 20 nA and the beam diameter was 10 μm . At these operating conditions, no intensity change due to sample damage was observed. Peak intensities were counted for 20 s and backgrounds were calculated using a mean atomic number correction (Donovan *et al.*, 2011). The following lines and standards were used for quantification: albite for NaK α ; diopside for MgK α and CaK α ; sanidine for KK α and AlK α ; hematite for FeK α ; rutile for TiK α ; tephroite for SiK α and MnK α ; sanbornite for BaL α ; and chromite for CrK α . Raw intensities were converted to concentrations using the default $\phi\rho Z$ corrections of the *Probe for EPMA* software (c.f. Armstrong, 1988). Results of microprobe analyses are presented in Table 2. The final chemical formulae (Table 1) are calculated for each analyses on the basis of 9 anions per formula unit

(apfu); H₂O (wt.% oxide) was calculated on the basis of stoichiometry, with (OH) = 1 apfu.

Powder X-ray diffraction

X-ray diffraction data (Table 3) for schizolite NHMD 1899.856 were acquired with a Bruker D8 discover equipped with CuK α radiation and a Deskris Eiger2R_500K detector, calibrated at a distance of 17.562 cm using a statistical calibration (Rowe, 2009). Schizolite, as expected, is characterised by an intermediate diffraction pattern between end-members of the pectolite-serandite series. The unit cell was refined in the triclinic system, based on the powder data, thanks to the increased detector resolution and the flexibility the Rietveld software for cell-refinement purposes. The recent improvement in data resolution and area detection technology facilitates the characterisation of lower symmetry structure, for which accurate pattern indexing was historically difficult and often impossible.

The discrepancy between the measured and calculated intensities in Table 3, largely result from the inability of the diffraction experiment to resolve the high-intensity peaks at $d = 2.8779$ and $d = 2.8725$ Å, corresponding to *hkl* indices (120) and (220), respectively. The (120) is the maximum (100%) peak in the calculated powder pattern, whereas (220) is calculated to be 93% of this intensity. As the 100% reference in the experimental pattern consists of both calculated peaks, the observed peak intensities are systematically, proportionally lower than predicted. Accounting for this would result in a better match between observed and calculated data.

Single-crystal X-ray diffraction data and structure refinement

Two crystal-structure analyses on schizolite were carried out. In both cases, single crystals were fixed to glass fibres and a Bruker single-crystal diffractometer equipped with an APEX II area detector and a microfocus sealed X-ray tube operating at 50 kV and 0.99 mA, located at the X-ray Crystallography Laboratory at the University of British Columbia (Vancouver, Canada), was used for the collection of intensity data. In all cases, data were collected with MoK α radiation at 293(2) K and measured φ and ω scans of 0.5° per frame. The *APEX III* software package was used to determine a data collection strategy that ensured complete coverage of the Ewald Sphere with reasonable data redundancy. The program *SAINT* (V3.38, Bruker, 2013) was used to index and refine the final unit-cell parameters, as well as reduce, scale and apply an adsorption correction.

Non-merohedral twinning was observed in sample NHMD 1899.856. Using *CELL_NOW* (V. 2008/4; Sheldrick, 2008), more than two domains were found; these were verified visually using the *RLATT* routine available in the *APEX III* software package. Only the two most prominent domains (rotated 2.9° about the **b** axis) were used during the integration routine. The structure was refined on a merged data set of the two domains. *TWINABS-2012/1* (Bruker, 2012) was used to calculate a multi-scan absorption correction. The twinned structure was solved against an *HKLF4* file, containing reflection intensities averaged over the two twin domains, and was refined again with a *HKLF5* file, containing domain-separated data. No twinning was observed in the data for sample NHMD 1899.8.

For the crystal taken from NHMD 1899.856, the structure was solved with Direct Methods using *SHELXS-97* (Sheldrick, 1997)

Table 5. Final refined atomic coordinates, site-occupancy factors (s.o.f.) and thermal parameters for schizolite Tutop Agtakörfia, Greenland (NHMD 1899.856).

Site	x/a	y/b	z/c	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}	U_{eq}	BVS
Na1	0.55613(2)	0.24495(3)	0.34892(2)	0.00918(5)	0.01998(7)	0.01896(6)	-0.00059(6)	0.00339(5)	-0.00031(5)	0.01649(4)	1.25
M1*	0.84858(2)	0.59389(2)	0.14628(2)	0.00732(2)	0.00598(2)	0.00780(2)	0.00069(1)	0.00110(1)	0.00143(1)	0.00702(1)	1.86
M2*	0.85187(2)	0.08497(2)	0.13471(2)	0.00752(2)	0.00785(2)	0.00999(2)	0.00060(1)	0.00081(1)	0.00243(1)	0.00833(1)	1.99
Si1	0.21976(2)	0.40698(2)	0.33595(2)	0.00671(3)	0.00527(3)	0.00625(3)	0.00025(2)	0.00004(2)	0.00194(2)	0.00601(2)	3.98
Si2	0.20668(2)	0.96031(2)	0.34935(2)	0.00615(3)	0.00488(3)	0.00730(3)	-0.00011(2)	-0.00001(2)	0.00132(2)	0.00613(2)	3.96
Si3	0.45065(2)	0.74640(2)	0.14303(2)	0.00512(3)	0.00626(3)	0.00675(3)	-0.00007(2)	0.00066(2)	0.00135(2)	0.00603(2)	3.88
O1	0.65702(3)	0.80673(4)	0.12209(4)	0.00638(7)	0.01074(8)	0.01444(9)	0.00092(7)	0.00271(7)	0.00168(6)	0.01046(5)	1.99
O2	0.32577(3)	0.72349(3)	-0.05592(3)	0.00974(8)	0.01180(8)	0.00816(8)	-0.00052(7)	-0.00157(7)	0.00151(7)	0.01017(5)	2.20
O3	0.19138(3)	0.50991(3)	0.53878(3)	0.01394(8)	0.00946(8)	0.00715(8)	-0.00106(6)	0.00100(7)	0.00502(6)	0.00981(4)	1.92
O4	0.15573(3)	0.85336(3)	0.54966(4)	0.01556(9)	0.00795(8)	0.00977(8)	0.00222(7)	0.00421(7)	0.00244(7)	0.01094(5)	1.95
O5	0.06066(3)	0.38523(4)	0.17145(3)	0.00793(7)	0.01225(8)	0.00753(7)	0.0006(7)	-0.00048(6)	0.00309(6)	0.00917(4)	2.00
O6	0.05645(3)	0.90371(4)	0.17321(4)	0.00846(8)	0.01017(8)	0.01059(8)	-0.00107(7)	-0.00240(7)	0.00102(6)	0.01009(5)	1.96
O7	0.40377(3)	0.53328(3)	0.25622(4)	0.00891(8)	0.00832(8)	0.01556(9)	0.00423(7)	0.00318(7)	0.00177(6)	0.01080(5)	1.91
O8	0.39139(3)	0.90471(3)	0.29269(4)	0.00859(7)	0.01018(8)	0.01185(8)	-0.00321(7)	0.00106(7)	0.00399(6)	0.00994(4)	2.15
O9	0.26533(3)	0.19699(3)	0.39234(3)	0.00959(7)	0.00457(7)	0.01207(8)	0.00040(6)	-0.00028(7)	0.00207(6)	0.00873(4)	2.26
H1	0.157(1)	0.670(1)	0.536(1)	*0.05							1.26

M1* s.o.f. Ca 0.792(1) and Mn 0.208(1); M2* s.o.f. Ca 0.792(1) and Mn 0.208(1)
 U_{iso} parameter fixed during refinement; BVS – bond-valence sum.

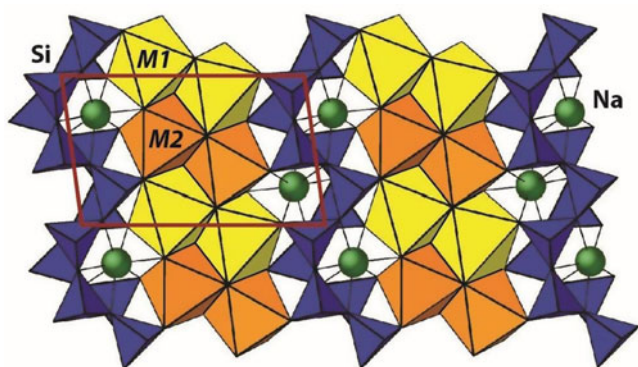


Fig. 2. The schizolite crystal structure. It shows the tri-periodic $[\text{Si}_3\text{O}_{10}]$ chains that zigzag parallel to c between double-wide ribbons of edge-sharing octahedra. The ribbon is formed by dimers of M1 (yellow) and M2 (orange) octahedra.

and refined by the Least Squares Method using version 2014 of *SHELXL* (Sheldrick, 2015). For the crystal taken from NHMD 1899.8, the structure was refined against the structure presented in Ohashi and Finger (1978). The transformation matrix from Ohashi and Finger (1978) to our cell is $[-\frac{1}{2}-\frac{1}{2}0 / 00-1 / -\frac{1}{2}-\frac{1}{2}0]$. The M1 and M2 sites were refined with split-occupancies (with the constraint $\text{Mn} + \text{Ca} = 1$). All positions were refined anisotropically, with the exception of hydrogen ($U_{iso} = 0.05 \text{ \AA}^2$), which, in all cases was readily observed in the difference-Fourier prior to being included in the refined model. The O–H distance was allowed to refine freely to O3–H1 = 1.22(1), O4–H1 = 1.28(1) and O3–H1...O4 = 2.4726(4) Å. Scattering factors of neutral atoms were taken from the *International Tables for X-ray Crystallography* (Ibers and Hamilton, 1974). For all crystals, assigning phases to a set of normalised structure-factors gave mean values of $|E^2 - 1|$ in excess of 0.95, in accord with a centrosymmetric space-group. Weighting parameters were manually updated during final Least Square cycles, and this process was repeated until convergence. For sample NHMD 1899.856, details of collection and refinement are given in Table 4, and final atomic coordinates are given in Table 5; structural formulae, calculated by site-refinement are given in Table 1. Compatible structure data for sample NHMD 1899.8 have been deposited as

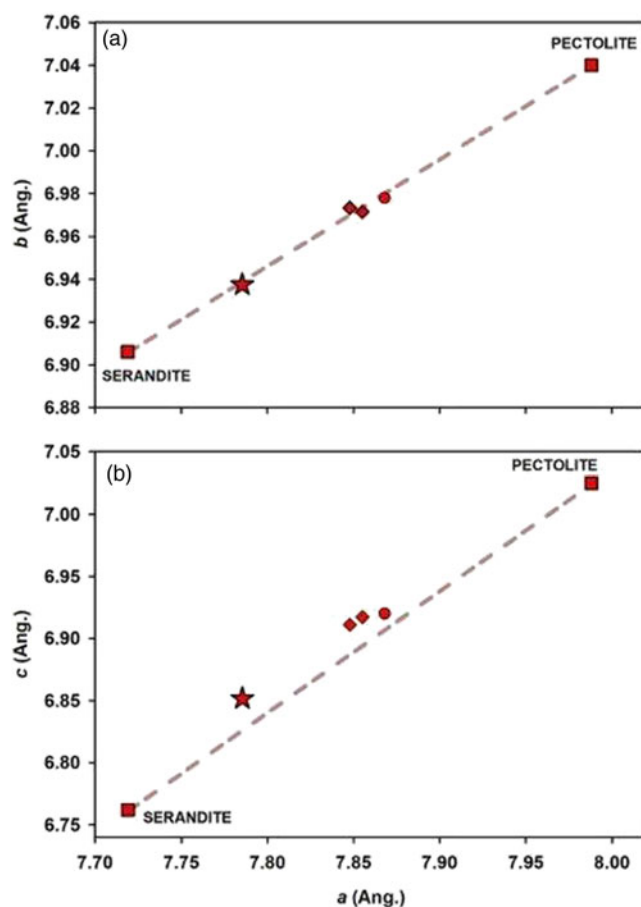


Fig. 3. Variation in unit-cell parameters for serandite (Jacobson *et al.*, 2000) and pectolite (Prewitt, 1967). The data of Ohashi and Finger (1978) (circle), this study (diamond) and ‘marshallsussmanite’ (star) are plotted for comparison: (a) a vs. b cell parameter; (b) a vs. c parameter.

supplementary material (see below). The final structure is entirely consistent with previously reported intermediate compositions of the serandite–pectolite solid-solution series (Fig. 2). It shows the tri-periodic $[\text{Si}_3\text{O}_{10}]$ chains, *dreierinfach* chains that zigzag

parallel to *c* between double-wide ribbons of octahedra are made up of two crystallographically-unique octahedrally-coordinated sites, *M1* and *M2* (Fig. 2). The final structures for NHMD 1899.856 and NHMD 1899.8 are very similar, but not identical i.e. small differences in Mn²⁺ and Ca content but consistent in the ordering of the *M1* and *M2* sites. Summary data for four minerals are given in Table 1. Consistent with previous authors, (Nagashima *et al.*, 2018; Ohashi and Finger, 1978; Prewitt, 1967; Rozhdestvenskaya and Vasilieva, 2014) Ca and Mn preferentially order at *M1* and *M2*, respectively, resulting in the ideal structural formula for schizolite being written as Na^{(M1)Ca^(M2)Mn}Si₃O₈(OH).

Discussion

The unit cell and optical parameters, as well as calculated empirical chemical formulae for all phases of interest are listed in Table 1. Close inspection of these confirm the equivalence of schizolite and ‘marshallsussmanite’. In all cases, the values of these parameters fall between those of the series end-members, pectolite and serandite. Parameters for ‘marshallsussmanite’ are reasonably similar to those of the two schizolite samples presented here. The variation in unit-cell parameters for the phases presented in Table 1 is shown in Fig. 3. A clear, linear trend relates the variation in parameters for pectolite–schizolite–serandite. Data corresponding to schizolite (NHMD 1899.8 and NHMD 1899.856) and ‘marshallsussmanite’ all plot along the trend, centrally located between the end-member values. These observations are in-line with general expectations, as the composition of schizolite can be expressed as being equal parts of the two end-members.

Conclusions

Schizolite and ‘marshallsussmanite’ are the same mineral species (Table 1). As the mineral name schizolite was published first, it is this name that must be used. The name ‘marshallsussmanite’ has now been discredited (Voting proposal 18-B, Hålenius *et al.*, 2018). It is unfortunate that the name ‘marshallsussmanite’ is now in the literature and widely spread throughout mineral trade, having been sold under that name. Circumstances such as this exemplify why withholding the approved name of new minerals in advance of the official publication may be a useful consideration. The present authors greatly appreciate data of new minerals being published quickly to prevent overlap of research efforts.

Author ORCID.  Ralph Rowe, 0000-0002-8735-7592.

Acknowledgements. Theresa Smith, Mineralogical & Geological Museum at Harvard University, kindly provided information on the specimen used by Ohashi and Finger (1978) in the first structure determination of schizolite. We would like to thank the following individuals for the use of their single-crystal diffractometers: Anita Lam and Brian Patrick, X-ray Crystallography Facility – University of British Columbia. We further thank two reviewers and for their thoughtful reviews and comments on the manuscript.

Supplementary material. To view supplementary material for this article, please visit <https://doi.org/10.1180/mgm.2019.21>.

References

- Armstrong J.T. (1988) Quantitative analysis of silicate and oxide materials: Comparison of Monte Carlo, ZAF, and procedures. *Microbeam Analysis*, 239–246.
- Boggild O.B. (1903) On some minerals from the nepheline-syenite at Julianehaab, Greenland (erikite and schizolite). *Meddelelser om Grønland*, **26**, 91–139.
- Bruker (2012) *TWINABS-2012/1*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2013) *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Donovan J.J., Lowers H.A. and Rusk B.G. (2011) Improved electron probe microanalysis of trace elements in quartz. *American Mineralogist*, **96**, 274–282.
- Flink G. (1898) Berättelse om en mineralogisk resa i Syd- Grønland sommeren 1897. *Meddelelser om Grønland*, **14**, 221–262.
- Hålenius U., Hatert F., Pasero M. and Mills S.J. (2018) IMA Commission on New Minerals, Nomenclature and Classification, Newsletter 43. *Mineralogical Magazine*, **82**, pp. 781–787.
- Ibers J.A. and Hamilton W.C. (1974) *International Tables for X-ray Crystallography*. The Kynoch Press, Birmingham, UK.
- Jacobsen S.D., Smyth J.R., Swope R.J. and Sheldon R.I. (2000) Two proton positions in the very strong hydrogen bond of serandite. *American Mineralogist*, **85**, 745–752.
- Lacroix A. (1931) Les pegmatites de la syénite sodalitique de l’îleRouma. Description d’un nouveau minéral (serandite) qu’elles renferment. *Compte Rendus Académie Science Paris*, **192**, 197–194.
- Nagashima M., Imaoka T., Fukuda C. and Pettke T. (2018) Relationship between cation substitution and hydrogen-bond system in hydrous pyroxenoids with three-periodic single-chains of SiO₄ tetrahedra: pectolite, murakamiite, marshallsussmanite, serandite and tanohataite. *European Journal of Mineralogy*, **30**, 451–463.
- Ohashi Y. and Finger L.W. (1978) The role of octahedral cations in pyroxenoid crystal chemistry. I. Bustamite, wollastonite, and the pectolite-schizolite-serandite series. *American Mineralogist*, **63**, 274–288.
- Origlieri M.J., Downs R.T. and Yang H. (2013) Marshallsussmanite, IMA 2013-067. CNMNC Newsletter No. 18, December 2013, page 3256; *Mineralogical Magazine*, **77**, 3249–3258.
- Origlieri M.J., Downs R.T., Yang H., Hoffman D.R., Ducea M.N. and Post J. (2017) Marshallsussmanite, NaCaMnSi₃O₈(OH), a new pectolite-group mineral providing insight into hydrogen bonding in pyroxenoids. *Mineralogical Magazine*, preproof [DOI <https://doi.org/10.1180/minmag.2017.081.049>].
- Petersen O.V. and Johnsen O. (2005) *Mineral Species First Discovered from Greenland*. Canadian Mineralogist, Special Publication, **8**. Mineralogical Association of Canada, Quebec, Canada.
- Prewitt C.T. (1967) Refinement of the structure of pectolite, Ca₂NaHSi₃O₉. *Zeitschrift für Kristallographie* **125**, 298–316.
- Rowe R. (2009) New statistical calibration approach for Bruker AXS D8 Discover microdiffractometer with Hi-Star detector using GADDS software. *Powder Diffraction* **24**, 263–271.
- Rozhdestvenskaya I.V. and Vasilieva V.A. (2014) Cation ordering and structural deformations in pectolite HNaCa₂Si₃O₉ – serandite HNaMn₂Si₃O₉. *Journal of Structural Chemistry*, **55**, 1268–1276.
- Schaller W.T. (1955) The pectolite-schizolite-serandite series. *American Mineralogist*, **40**, 1022–1031.
- Sheldrick G.M. (1997) *SHELXS-97 and SHELXL-97, Program for Crystal Structure Solution and Refinement*. University of Göttingen, Göttingen, Germany.
- Sheldrick G.M. (2008) *CELL_NOW*. Version 2008/4. Georg-August-Universität Göttingen, Göttingen, Germany.
- Sheldrick G.M. (2015) *SHELXL* Version 2014. *Acta Crystallographica*, **C71**, 3–8.
- Winther C. (1901) Schizolite, a new mineral. *Meddelelser om Grønland*, **24**, 196–203.