

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

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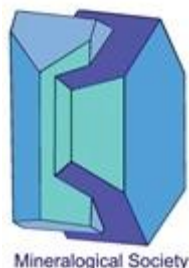
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ABSTRACT

Schizolite, originating from the type locality, Tutop Agtakôrfia, in the Ilímaussaq alkaline complex, Julianehåb district, South Greenland, was initially described 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 (IMA 2013-067) by Origlieri *et al.* (2013). Results from the detailed examination of two schizolite cotype samples presented here, using single-crystal XRD, powder XRD, and optics, confirms it 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,



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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 positive, 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: SiO₂, 52.6(4); Al₂O₃, 0.005(1); FeO, 2.54(2); MnO, 13.86(9); CaO, 17.9(4); Na₂O 8.9(1); H₂O, 2.59(2) wt. % oxide; this corresponds to a mean formula of: Na_{1.00(2)}Ca_{1.11(7)}Mn_{0.68(1)}Fe_{0.12(0)}Si_{3.041(1)}O₈(OH). Final least-squares structure refinements for both samples converged at R_1 -values $\leq 2.0\%$; H atoms were located in all refinements.

Introduction

The new mineral proposal for “marshallsussmanite” (2013-067) 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. Since then, Nagashima *et al.* (2018) refined the structure of a “marshallsussmanite”.

In this brief account, we have re-characterized the cotype material from Tutop Agtakôrfia, 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). 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 characterization

The type locality of schizolite is Tutop Agtakôrfia (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 Agtakôrfia 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 (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 $\text{Na}(\text{Ca},\text{Mn})_2\text{Si}_3\text{O}_8(\text{OH})$. 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 ($\text{Na}^{M1}\text{Ca}^{M2}\text{CaSi}_3\text{O}_9\text{H}$), schizolite ($\text{Na}^{M1}\text{Ca}^{M2}\text{MnSi}_3\text{O}_9\text{H}$), and serandite ($\text{Na}^{M1}\text{Mn}^{M2}\text{MnSi}_3\text{O}_9\text{H}$). However, these authors did not emphasize 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.

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 G. Flink in 1897 (Fig. 1a). This specimen is part of a suite of 14 specimens studied by Winther, with an additional 7 that were also likely 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 and the Natural History Museum in Oslo. 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 in length. 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) ~ 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 positive 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 positive 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 specimens. Optical parameters were measured on a crystal fragment using a spindle stage with Na light, $\lambda = 590$ nm and the measured 2V is 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. 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 seconds 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 Na $K\alpha$, diopside for Mg $K\alpha$, Ca $K\alpha$, sanidine for K $K\alpha$, Al $K\alpha$, hematite for Fe $K\alpha$, rutile for Ti $K\alpha$, tephroite for Si $K\alpha$, Mn $K\alpha$, sanbornite for Ba $L\alpha$, and chromite for Cr $K\alpha$. Raw intensities were converted to concentrations using the default Phi-Rho-Z corrections of the Probe for EPMA software (<https://probesoftware.com> and *cf* 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 *pfu*; H₂O (wt. % oxide) was calculated on the basis of stoichiometry, with (OH) = 1 *pfu*.

X-ray powder diffraction

X-ray diffraction data (Table 3) for schizolite NHMD 1899.856 were acquired with a Bruker D8 discover equipped with $\text{CuK}\alpha$ 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 characterized 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 characterization 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 $d = 2.8779 \text{ \AA}$ and $d = 2.8725$, corresponding to hkl 's (120) and (2-20), respectively. The (120) is the maximum (100%) peak in the calculated powder pattern, whereas (2-20) 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, 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 $\text{MoK}\alpha$ 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 (Bruker, V3.38 - 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 1890.856, the structure were solved with Direct Methods using SHELXS-97 (Sheldrick, 1997) and refined by the Least Squares Method using version 2014 of XL (Sheldrick, 2015). For 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 $Mn + Ca = 1$). 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 be 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 taken from the International Tables for X-ray Crystallography (Ibers & Hamilton 1974). For all crystals, assigning phases to a set of normalized 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 5, and final atomic coordinates are given in Table 6; structural formulae, calculated by site-refinement are given in Table 1. Compatible structure data for Sample NHMD 1899.8 have been deposited as supplementary material. The final structure is entirely consistent with previously reported intermediate compositions of the serandite-pectolie solid solution series. 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*. The final structures for NHMD 1899.856 and NHMD 1899.8 are very similar, but not identical *i.e.* small differences in Mn^{2+} and Ca content but consistent in the ordering of the *M1* and *M2* sites. Summary data for the 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 is written as $\text{Na} (^{M1}\text{Ca}^{M2}\text{Mn})\text{Si}_3\text{O}_8(\text{OH})$.

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. Figure 4 shows the variation in unit cell parameters for the phases presented in Table 1. 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 (International Mineralogical Association, Commission on New Minerals, Nomenclature and Classification Memorandum 85-FH/18). 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 quickly published to prevent overlap of research efforts.

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.

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Figure 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

Figure 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.

Figure 3.

Variation in unit cell parameters for serandite (Jacobson *et al.* 2000) and pectolite (Prewitt, 1967). The data of Ohashi & Finger (1971) (circle), this study (diamond), and ‘marshallsussmanite (star) are plot for comparison. In (a) a vs. b cell parameter, in (b) a vs. c parameter.

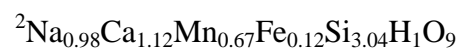
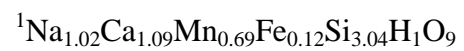
Table 1. Comparison of schizolite, ‘marshallsusmanite’, serandite and pectolite

Mineral species (data reference)	SERANDITE	SCHIZOLITE	‘MARSHASUSSM ANITE’	SCHIZOLITE (NHMD 1899.856)	SCHIZOLITE (NHMD 1899.8)	PECTOLITE (Schaller, 1955; Prewitt, 1967)
Formula (ideal)	$\text{NaMnMnSi}_3\text{O}_8(\text{OH})$	$\text{NaCaMnSi}_3\text{O}_8(\text{OH})$	$\text{NaCaMnSi}_3\text{O}_8(\text{OH})$	$\text{NaCaMnSi}_3\text{O}_8(\text{OH})$	$\text{NaCaMnSi}_3\text{O}_8(\text{OH})$	$\text{NaCaCaSi}_3\text{O}_8(\text{OH})$
Formula (empirical)	$\text{Na}_{0.88}\text{Mn}_{1.47}\text{Ca}_{0.67}\text{Si}_{2.9}$ $_{3}\text{O}_9\text{H}_{1.06}^{\text{B}}$	$\text{Na}_{1.07}\text{Ca}_{1.21}\text{Mn}_{0.63}\text{Fe}_0$ $_{.14}\text{Si}_{2.93}\text{O}_9\text{H}_{0.53}^{\text{B}}$	$\text{Na}_{0.91}\text{Ca}_{0.96}\text{Mn}_{1.07}\text{Si}_3$ $_{01}\text{O}_9\text{H}$	$\text{Na}(\text{Ca}_{0.917}\text{Mn}_{1.08})$ $\text{Si}_3\text{O}_9\text{H}$	$\text{Na}(\text{Ca}_{0.96}\text{Mn}_{1.04})$ $\text{Si}_3\text{O}_9\text{H}$	$\text{Na}_{0.97}\text{Ca}_{1.98}\text{Si}_{2.97}\text{O}_9\text{H}$ $_{1.20}^{\text{A}}$
Formulae (SREF)	--	--	$(\text{Na}_{0.948}\text{Li}_{0.052})$ $^{\text{M1}}(\text{Ca}_{0.793}\text{Mn}_{0.207})$ $^{\text{M2}}(\text{Ca}_{0.937}\text{Mn}_{0.063})$ $\text{Si}_3\text{O}_8(\text{OH})$	$\text{Na}^{\text{M1}}(\text{Ca}_{0.734}\text{Mn}_{0.266})$ $^{\text{M2}}(\text{Mn}_{0.817}\text{Ca}_{0.183})$ $\text{Si}_3\text{O}_8(\text{OH})$	$\text{Na}^{\text{M1}}(\text{Ca}_{0.772}\text{Mn}_{0.228})$ $^{\text{M2}}(\text{Mn}_{0.813}\text{Ca}_{0.187})$ $\text{Si}_3\text{O}_8(\text{OH})$	--
Physical properties	Bladed, salmon-red ^A	Prismatic, pink to	Bladed, orange-	Pale pink	Pale brown	Prismatic, colourless

	Peach ^B	brown ^B	tinted pink			to white ^{A,B}
Density (gcm ⁻³)	3.34 ^A	3.05 ^A	3.17			2.90 ^A
Optical properties (α , β , γ , 2V°)	1.668, 1.671, 1.703, 39 ^A	1.631, 1.636, 1.660, 47 ^A	1.641, 1.646, 1.671, 49	1.626(3) 1.630(2) 1.661(2) 72(4)	1.640(3) 1.643(2) 1.658(2) 52(2)	1.610, 1.615, 1.643, 53 ^A
Space Group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
Cell parameters (a , b , c , Å)	7.719, 6.906, 6.762, 90.50, 94.09, 102.78,	7.868, 6.978, 6.920 90.72, 94.53,	7.783, 6.937, 6.850, 90.68, 94.33,	7.8551(2), 6.9715(2), 6.9173(2)	7.8492(1), 6.9752(1),	7.988, 7.040, 7.025, 90.52, 95.18, 102.47,
(α , β , γ , °), (V , Å ³)	350.6 ^B	102.92, 366.4 ^B	102.85, 359.4	90.756(1), 94.489(1), 102.858(1), 367.99(1)	6.9117(1), 90.791(1), 94.452(1), 102.849(1), 367.64(1)	384.0 ^B
Sample Locality	Rouma Isle, Guinea ^A Mont Saint-Hillaire, Canada ^B	Kangerdluarssuk, Greenland	Wessels mine, South Africa	Tutop, Agtakôrfia, Greenland.	Tutop, Agtakôrfia, Greenland.	Lovozero, Russia ^A Bergen Hill, New Jersey ^B
References	A. Lacroix, 1931; B. Jacobsen <i>et al.</i> 2000	A. Schaller, 1955; B. Ohashi and Finger, 1978	Origlieri <i>et al.</i> , 2013	This study.	This study.	A. Schaller, 1955; B. Prewitt, 1967

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

Sample no.	NHMD 1899.856 ¹		NHMD 1899.8 ²	
Mineral Species	schizolite (cotype)		schizolite (cotype)	
	26 analyses		21 analyses	
Av. Wt.%, range	Wt.%	range	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 O*	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



Atomic fractions calculated of the basis of 9 oxygen atoms

* H₂O calculated on the basis of 1 H apfu

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

<i>I</i> obs.	<i>I</i> calc. *	<i>d</i> obs.	<i>d</i> calc. *	hkl
12	15	7.624	7.6261	100
11	14	6.884	6.8866	001
	5		6.7940	010
4	5	5.338	5.3378	-101
2	2	4.908	4.9121	0-11
4	7	4.590	4.5868	110
3	6	4.499	4.4995	-111
2	4	4.339	4.3377	1-11
5	9	3.951	3.9489	-1-11
13	18	3.813	3.8131	200
3	2	3.700	3.6987	2-10
9	13	3.443	3.4433	002
3	2	3.394	3.4000	1-20
	3		3.3970	020
4	4	3.348	3.3497	-221
34	48	3.241	3.2415	-102
26	32	3.225	3.2236	201
12	16	3.111	3.10999	0-12
	2		3.0456	210
42	58	3.047	3.0443	102
50	16	3.044	3.0342	012
15	25	3.005	3.0045	-112
4	9	2.910	2.908	1-12
100	93	2.875	2.8779	2-20
	100		2.8725	120
	4		2.8724	-2-11
	2		2.8525	-1-12
6	12	2.707	2.7068	-1-21
4	9	2.692	2.6912	-221
12	23	2.670	2.6689	-202
6	11	2.579	2.5786	3-10
14	26	2.543	2.5420	300
3	2	2.455	2.4561	0-22
	3		2.4555	202
9	2	2.412	2.4275	-122

	19		2.4113	1-22
8	15	2.381	2.3821	022
15	14	2.296	2.2980	3-20
	6		2.2955	003
	8		2.2934	220
	3		2.2707	-1-22
19	27	2.251	2.2507	-103
	3		2.2497	-222
3	5	2.221	2.2226	310
4	3	2.196	2.1954	212
	2		2.1952	0-13
3	3	2.170	2.1685	-3-11
8	14	2.146	2.1448	3-21
12	7	2.132	2.1320	-302
	16		2.1311	221
4	3	1.9085	1.9085	-2-13
	2		1.9084	-123
	3		1.9065	400
	2		1.8966	1-23
2		1.8779	1.8782	-401
			1.8756	023
2		1.8664	1.8661	032
			1.8647	3-22
3	4	1.8504	1.8532	-232
	5		1.8492	232
3	4	1.8287	1.8280	-223
2	3	1.8204	1.8228	2-32
	2		1.8186	-3-21
	5		1.8009	-1-32
	4		1.7992	401
3	4	1.7572	1.7629	2-23
	4		1.7579	4-21
	4		1.7496	321
	3		1.7451	123
10	28	1.7431	1.7431	1-40
	3		1.7369	410
7	13	1.7215	1.7217	004
8	6	1.6829	1.6832	-2-23
	13		1.6820	-3-22
6	15	1.6749	1.6748	-422
3	5	1.6702	1.6705	-323
2	5	1.6367	1.6370	303
2	4	1.6215	1.6208	-204
2	7	1.5876	1.5872	4-22
3	6	1.5775	1.5770	322

3	9	1.5418	1.5421	0-42
2	4	1.5266	1.5309	-403
	4		1.5284	-242
	4		1.5254	5-20
2	3	1.5230	1.5229	420
2	2	1.5166	1.5203	2-42
	2		1.5171	024
	2		1.5161	-501
	2		1.5155	-1-24
4	10	1.4638	1.4635	501
5	12	1.4536	1.4535	2-24
6	12	1.4406	1.4408	124
2	5	1.3731	1.3732	304
4	3	1.3535	1.3534	-2-42
	5		1.3533	502

*Calculated from structure data modified with XRPD Rietveld 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

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Table 4. Schizolite, Tutop Agtakôrfia NHMD 1899.856 (cotype), Greenland

Space Group	$P\bar{1}$ (SG # 2)	Measured reflections	17034
a (Å)	7.8551(2)	α° 90.756(1)	Unique reflections 3588
b (Å)	6.9715(2)	β° 94.489(1)	Observed reflections [$> 4\sigma(F)$] 3443
c (Å)	6.9173(2)	γ° 102.858(1)	$R(\text{int})$ 0.014
V (Å ³)	367.99(1)	Goodness of fit on F^2	0.955
Range of reflections, hkl	$\pm 13 / \pm 11 / \pm 11$	R index for all data	0.015
Number l.s. parameters	150	R index for observed data	0.014
$F(000)$	347.0	wR^2 for all data	0.044

Ideal unit-cell contents: 2[NaCaMnSi₃O₉H] $\mu = 3.54 \text{ mm}^{-1}$

Refinement by full-matrix least squares on F^2

$$R1 = \sum | |F_{obs}| - |F_{calc}| | / \sum |F_{obs}| ; wR2 = \left[\sum [w(F_{obs}^2 - F_{calc}^2)^2] / \sum w(F_{obs}^2)^2 \right]^{1/2}$$

$$Goof = \left[\sum [w(F_{obs}^2 - F_{calc}^2)^2] / (n - p) \right]^{1/2}$$

$$w = 1 / [\delta^2(F_0^2) + (0.0269 \times P)^2 + 0.20 \times P] \text{ where } P = (\text{Max}(F_0^2, 0) + F_c^2) / 3$$

TABLE 6. Final refined atomic coordinates, site-occupancy factors, and thermal parameters for schizolite Tutop Agtakôrfa, Greenland (NHMD 1899.856)

Site	Occ. Fac.	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ²³	<i>U</i> ¹³	<i>U</i> ¹²	<i>U</i> _{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
<i>M1</i> *	Mn _{0.208} Ca _{0.792}	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
<i>M2</i> *	Mn _{0.786} Ca _{0.214}	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

M(1)* Ca sof 0.792(1), Mn sof 0.208(1)

M(2)*Ca sof 0.214(1), Mn sof 0.786(1)

*U*_{iso} parameter fixed during refinement.

Figure 1a: Schizolite collected by Gustaf Flink in 1897 and used in the original description by Christian Winther (1901); catalogue NHMD 1899.856



Sample #1899.856 Natural History Museum of Denmark, Geological Museum

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Figure 1b: Schizolite collected by Ove Balthasar Bøggild and Brunnurstedt in 1899; catalogue NHMD 1899.8

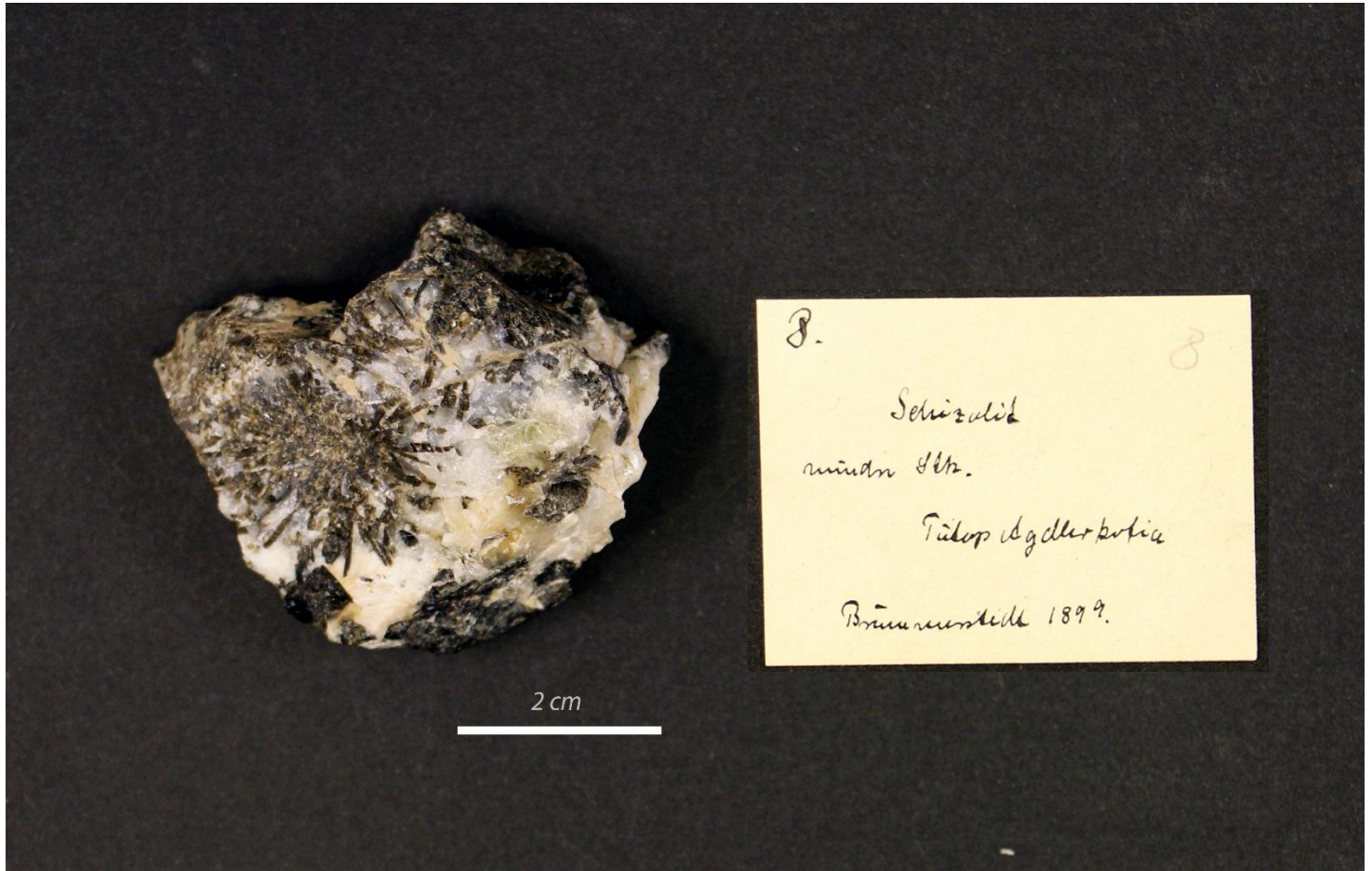
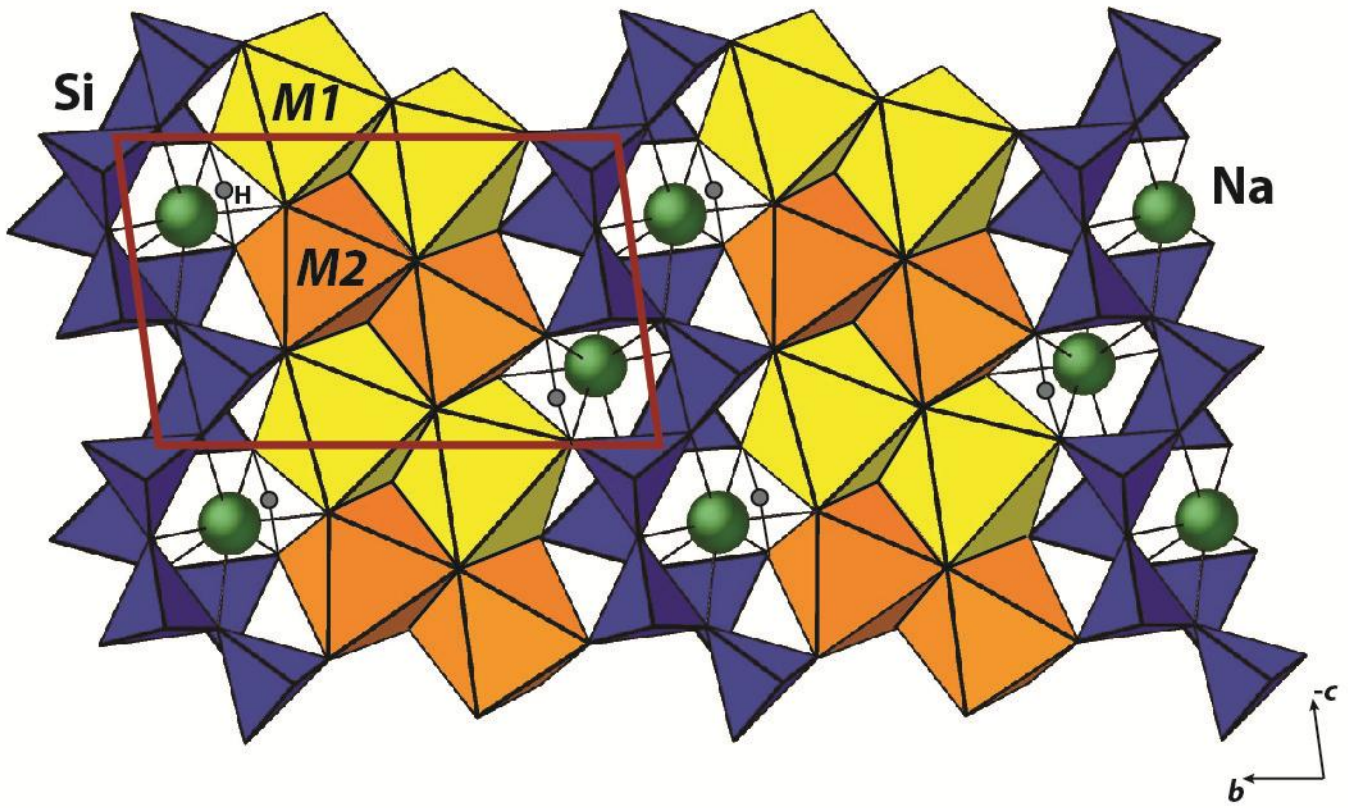


Figure 2.

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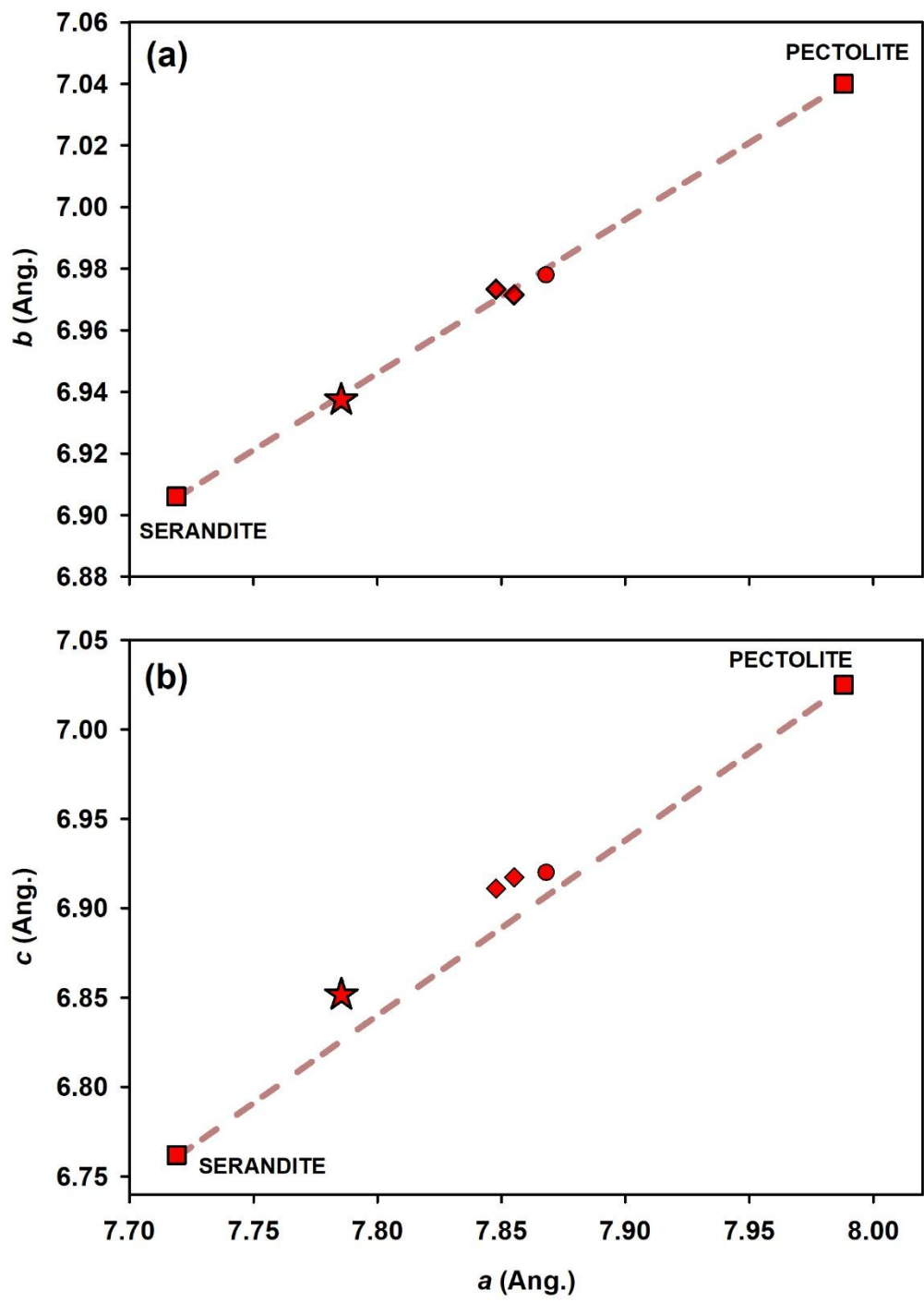


FIGURE 3