1	Revision 1
2	Eckermannite revised. The new holotype from the Jade Mine Tract,
3	Myanmar: crystal structure, mineral data and hints on the reasons for
4	the rarity of eckermannite
5	
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16	
17	Abstract
18	Following the characterization of the new amphibole species fluoro-leakeite, ideally ${}^{A}Na {}^{B}Na_{2}$
19	^C (Mg ₂ Al ₂ Li) ^T Si ₈ O ₂₂ ^W F ₂ , at Norra Kärr (Sweden), so far considered the type locality of eckermannite,
20	re-examination of the holotype material of eckermannite deposited at the Museum of Natural History in
21	London (BM 1949.151) and of the original sample analyzed by Törnebohm (1906) confirmed that they
22	both are actually fluoro-leakeite. A survey of literature data showed that the only analysis reported for
23	eckermannite is that of sample AMNH 108401 from the Jade Mine Tract, Myanmar. Complete 1

24	characterization of that sample has led to the approval of a new holotype for eckermannite (IMA-
25	CNMMC 2013-136), ideally ^A Na ^B Na ₂ ^C (Mg ₄ Al) ^T Si ₈ O_{22} ^W (OH) ₂ , which is described in this work.
26	Holotype eckermannite from Myanmar has the empirical unit formula $^{A}(Na_{0.87}K_{0.06})_{\Sigma=0.93}$
27	${}^{B}(Na_{1.89}Ca_{0.11})_{\Sigma=2.00} {}^{C}(Mg_{3.87}Fe^{2+}{}_{0.09}Mn_{0.01}Fe^{3+}{}_{0.38}Al_{0.62})_{\Sigma=4.97} {}^{T}Si_{8.00} O_{22} {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00}. \ It \ is$
28	monoclinic, $C2/m$, with $a = 9.8087(7)$, $b = 17.8448(13)$, $c = 5.2905(4)$ Å, $\beta = 103.660(1)$, $V = 899.8(1)$
29	Å ³ ; $Z = 2$, $D_{calc} = 3.02$ g/cm ³ . Optics: biaxial (–); α 1.605, β 1.630, γ 1.634 all ± 0.002 (λ = 590 nm).
30	The ten strongest reflections in the X-ray powder pattern [d values (in Å), I, (hkl)] are: 2.702, 100, [(-
31	331) (151)]; 3.395, 59, (131); 3.128, 56, (310); 2.525, 56, (-202); 8.407, 42, (110); 2.574, 36, [(061)
32	(002)]; 3.257, 34, (240); 2.161, 33, (261); 2.966, 33, (060); 4.460, 30, (040).
33	The reason for the rarity of eckermannite compositions are examined and discussed based on
34	considerations on the short-range order of A cations and W anions.
35	
36	Keywords: eckermannite, new holotype, amphibole, chemical analysis, crystal structure, Myanmar
37	
38	INTRODUCTION
39	Eckermannite is a "grandfathered" amphibole end-member with ideal formula $^{A}Na {}^{B}Na_{2}$
40	C (Mg ₄ Al) T Si ₈ O ₂₂ W (OH) ₂ , which was named after the Swedish petrologist Claes.V.H. (Harry) von
41	Eckermann (1886-1969). The name was proposed by Adamson (1942) based on the study of rock
42	samples from Norra Kärr, Gränna, Jönköping, Småland, Sweden. According to Holtstam (1998), the
43	Norra Kärr locality (58°06'N, 14°40'E) is a small oval Proterozoic alkaline intrusion, composed mainly
44	of fine-grained schistose agpaitic nepheline-syenite (grennaite). Petrological and genetic aspects of
45	Norra Kärr have been described extensively by Adamson (1944), von Eckermann (1968), Blaxland
46	(1977) and Kramm and Koark (1988). Adamson (1942) re-calculated the analyses of R. Mauzelius
47	reported (together with optical properties) in Törnebohm (1906), and recognized that this was a new
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48	amphibole species. It should be noted that a significant amount of Li (1.15 wt.% Li ₂ O, corresponding to
49	0.65 atoms per formula unit, apfu) was later reported in amphiboles from Norra Kärr by Sundius
50	(1945), who raised doubts on the composition of eckermannite. However, this did not result in re-
51	examination of the sample.
52	A few years ago, the study of a specimen from Norra Kärr in the collection of Renato and
53	Adriana Pagano showed the occurrence of a Li- and F-rich amphibole that was subsequently described
54	as fluoro-alumino-leakeite (IMA-CNMMNC 2009-012; Oberti et al., 2009), and became fluoro-
55	leakeite after Hawthorne et al. (2012). Based on the similarity of the published optical properties of
56	holotype eckermannite, that paper suggested that eckermannite did not occur at Norra Kärr. Re-
57	examination of the holotype specimen deposited at the Natural History Museum in London (BM
58	1949.151) and of the original material analyzed by Törnebohm (1906) (NRM 570725; courtesy of prof.
59	Ulf Hålenius, Stockholm) later confirmed this hypothesis, and showed that those samples are also
60	fluoro-leakeite.
61	Eckermannite is quite rare, and most of the available analyses of natural or synthetic samples
62	actually refer either to ferro-eckermannite or to fluoro-eckermannite (note that presently both these
63	species have the status of named amphiboles, so that their complete mineral descriptions have never
64	been reported). However, the rootname eckermannite was used by Hawthorne et al. (2012) to redefine
65	kozulite (IMA 1968-028; Nambu et al., 1969; formerly assigned by Leake et al., 1997) to mangano-
66	ferri-eckermannite based on the newly approved rules for amphibole classification and nomenclature.
67	Hence, it was not possible to discredit the root-name eckermannite. Instead of simply discrediting the
68	holotype material, we started a systematic characterization of the "eckermannite" samples published in
69	the literature. We found a specimen related to the ideal eckermannite composition only in the sample
70	from the collection of the American Museum of Natural History described in this work. After the

71	approval of IMA-CNMNC (vote 2013-136), the rock sample AMNH H108401 must be considered as
72	the holotype sample of eckermannite.
73	
74	MINERAL DATA
75	Occurrence and paragenesis
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77	The sample was extracted from a jadeitite-amphibole fels rock catalogued as AMNH H108401
78	in the mineral collection of the American Museum of Natural History, acquired in Myanmar by one of
79	us (GEH) in 2000. The rock consists of a boundary layer between mixed white and emerald green
80	jadeitite and a black amphibole fels, a sharp boundary separating the two parts. The rock was mined in
81	the Jade Mine Tract, Kachin Province, Myanmar. It is not known whether the rock comes from a
82	tectonic block in serpentinite or as part of a boulder extracted from the Uru River conglomerates
83	(Hughes et al., 2000). Associated minerals are jadeite and albite. All of the amphibole in this sample
84	falls within eckermannite-dominant compositions with $(Mg/(Mg+Fe^{2+}))$ between 0.84 and 1.
85	Amphibole fels adjacent to jadeitite from the Jade Mine Tract in Myanmar have been ascribed
86	to reactions between hydrous fluids that crystallized jadeitite and hosting serpentinized ultramafic
87	mantle wedge during subduction, but timing (whether jadeitite or fels formed first) is uncertain (Shi et
88	al., 2003, 2012). Conditions of formation in this high-pressure - low-temperature regime are not well
89	constrained, but are somewhere in the blueschist facies of metabasites, probably $300^{\circ}C < T < 400^{\circ}$ and
90	5 kbar $< P < 15$ kbar.
91	
92	Appearance, physical and optical properties

94	The amphibole fels is grey with white veins (Figure 1) and grains of eckermannite are
95	intergrown prisms generally less than 1 mm in maximum dimension. They are colorless to grey in
96	color, transparent, vitreous, and non-fluorescent. The tenacity is brittle and single crystals show a
97	perfect cleavage according {110}. The density calculated from the unit formula and cell dimensions is
98	3.02 g/cm^3 .
99	A spindle stage was used to orient a crystal for measurement of refractive indices and $2V$ by
100	extinction curves (Bartelmehs et al., 1992). The optical orientation was determined by transferring the
101	crystal from the spindle stage to a single-crystal diffractometer and measuring the relative axial
102	relations by X-ray diffraction. In transmitted light, eckermannite is biaxial negative with indices of
103	refraction $\alpha = 1.605$, $\beta = 1.630$, $\gamma = 1.634$ (all ± 0.002), measured with gel-filtered Na light ($\lambda = 589.9$
104	nm); $2V_{obs} = 43.0(5)$, $2V_{calc} = 43^{\circ}$. Orientation is $X^{\wedge} a = 23.8^{\circ}$ (in β obtuse), $Y \parallel b$, $Z^{\wedge} c = 10.1^{\circ}$ (in β
105	acute), and pleochroism is as follows: $X =$ medium grey (strongest), $Y =$ pale grey to colourless
106	(weakest), $Z = $ light grey (medium).
107	
108	Crystallography
109	
110	For samples AMNH H108401 (single crystal 120 x 60 x 40 μ m in size) and NMR 570725
111	(single crystal 200 x 160 x 60 μm in size), diffraction data were collected in the 20 range 2-60° with a
112	Bruker-AXS CCD diffractometer with graphite-monochromatized MoK α X-radiation ($\lambda = 0.7107$ Å).
113	For both crystals, omega-rotation frames (scan width 0.3°, scan time 20 s, sample-to-detector distance
114	50 mm) were processed with the SAINT software (Bruker, 2003) and intensities were corrected for
115	Lorentz and polarization effects; absorption effects were empirically evaluated by the SADABS
116	software (Sheldrick, 1996) and an absorption correction was applied to the data.

117	A total of 6891 reflections collected for sample AMNH H108401 was reduced to 1377 unique
118	reflections (mean redundancy = 5, R_{int} = 2.3%), and accurate unit-cell dimensions were calculated by
119	least-squares refinement of the positions of 1998 independent reflections with $I_0 > 10 \sigma I$ in the θ range
120	2-30°. For sample NMR 570725, 6580 collected reflections were reduced to 1321 unique reflections
121	(mean redundancy = 5, R_{int} = 1.3%), and accurate unit-cell dimensions were calculated by least-squares
122	refinement of the positions of 4074 independent reflections with $I_0 > 10 \sigma I$ in the θ range 2-30°.
123	For samples BM 1949.151, XRD analysis was done with a Philips PW1100 4-circle diffractometer ($\lambda =$
124	MoK α). Two monoclinic equivalents were collected in the 2 θ range 4-70°; corrections for absorption
125	and Lp were applied and 3960 collected data were merged to 2017 unique reflections ($R_{sym} = 2.2$ %).
126	Unit-cell parameters were calculated from least-squares refinement of the d* values obtained for 60 rows
127	of the reciprocal lattice by measuring the centre of gravity of each reflection and of its antireflection in the
128	2θ range -70° to 70° .
129	For all samples, only the reflections with $I_0 > 3 \sigma I$ were considered as observed during unweighted full-
130	matrix least-squares refinement on F done with a program locally written to handle complex solid-
131	solutions. Scattering curves for fully ionized chemical species were used at sites where chemical
132	substitutions occur; neutral vs. ionised scattering curves were used at the T and anion sites [except
133	O(3)]. More details on the refinement procedure and on the terminology used are given in Oberti et al.
134	(1992) and in Hawthorne et al. (1995). The $A(m)$ and $A(2)$ sites were inserted into the model to better
135	account for the irregular shape of the electron density within the A cavity, and testify to the presence of
136	significant ordering of the A cations. The absence of residual electron-density along the b direction at
137	around 0.40 Å from the $M(4)$ site (i.e., at the $M(4')$ site) indicates the absence of significant amounts of
138	smaller B cations (e.g., Li^+ , Fe^{2+} , Mg^{2+}).
139	The final values of R_{obs} and R_{all} are 2.9 and 4.0% for AMNH H188401, 1.6 and 2.6% for BM 1949.151,
140	and 2.1 and 2.3% for NMR 570725. Refined coordinates, atomic-displacement parameters, site

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141	occupancies and selected bond lengths and angles are given in Tables 1 and 2. Measured structure
142	factors have been deposited with the cif file.
143	X-ray powder-diffraction data (CuK α , λ = 1.54178 Å) for eckermannite AMNH H108401 were
144	calculated from the single-crystal data using the XPREP utility of SAINT (Bruker, 2003). No Lorentz
145	and polarization correction was applied. Data are given in Table 3.
146 147	EMP analysis
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149	Chemical analysis of the refined crystal of eckermannite (10 point analyses) was done with a
150	CAMECA SX-100 electron microprobe (WDS mode, 15 kV, 10 nA, 5 μ m beam diameter). The
151	following standards were used for Ka X-ray lines: Si: diopside, TAP; Ca: diopside, LPET; Ti: titanite,
152	LLiF; Fe: fayalite, LLiF; Mn: spessartine, LLiF; Cr: chromite, LLiF; Mg: forsterite, LTAP; Al:
153	andalusite, TAP; K: orthoclase, LPET; Na: albite, TAP; F: fluoro-riebeckite, LTAP. Zn, Cr and Cl
154	contents are below detection limits. H_2O was calculated from the unit formula to obtain 2 (OH + F) in
155	the absence of dehydrogenation, as indicated by the single-crystal structure refinement. The total Fe
156	content was first estimated as FeO; the ferrous and ferric populations were estimated later, imposing
157	electroneutrality and crystal-chemical constraints obtained from structure refinement. The results are
158	reported in Table 4. The empirical formula (based on 24 anions pfu) is $^{A}(Na_{0.87}K_{0.06})_{\Sigma=0.93}$
159	${}^{B}(Na_{1.89}Ca_{0.11})_{\Sigma=2.00} \ {}^{C}(Mg_{3.87}Fe^{2+}_{0.09}Mn_{0.01}Fe^{3+}_{0.38}Al_{0.62})_{\Sigma=4.97} \ {}^{T}Si_{8.00}O_{22} \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00}. \ The \ end-2000 \ Contract (Mg_{3.87}Fe^{2+}_{0.09}Mn_{0.01}Fe^{3+}_{0.38}Al_{0.62})_{\Sigma=4.97} \ {}^{T}Si_{8.00}O_{22} \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00}. \ The \ end-2000 \ Contract (Mg_{3.87}Fe^{2+}_{0.09}Mn_{0.01}Fe^{3+}_{0.38}Al_{0.62})_{\Sigma=4.97} \ {}^{T}Si_{8.00}O_{22} \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00}. \ The \ end-2000 \ Contract (Mg_{3.87}Fe^{2+}_{0.09}Mn_{0.01}Fe^{3+}_{0.38}Al_{0.62})_{\Sigma=4.97} \ {}^{T}Si_{8.00}O_{22} \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00}. \ The \ end-2000 \ Contract (Mg_{3.87}Fe^{2+}_{0.09}Mn_{0.01}Fe^{3+}_{0.38}Al_{0.62})_{\Sigma=4.97} \ {}^{T}Si_{8.00}O_{22} \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00}. \ The \ end-2000 \ Contract (Mg_{3.87}Fe^{2+}_{0.09}Mn_{0.01}Fe^{3+}_{0.38}Al_{0.62})_{\Sigma=4.97} \ {}^{T}Si_{8.00}O_{22} \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00}. \ The \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00} \ Contract (Mg_{3.87}Fe^{2+}_{0.09}Mn_{0.01}Fe^{3+}_{0.38}Al_{0.62})_{\Sigma=4.97} \ {}^{T}Si_{8.00}O_{22} \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00}. \ The \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00} \ Contract (Mg_{3.87}Fe^{2+}_{0.09}Mn_{0.01}Fe^{3+}_{0.38}Al_{0.62})_{\Sigma=4.97} \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00} \ Contract (Mg_{3.87}Fe^{2+}_{0.09}Mn_{0.01}Fe^{3+}_{0.38}Al_{0.62})_{\Sigma=4.97} \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00} \ Contract (Mg_{3.87}Fe^{2+}_{0.09}Mn_{0.01}Fe^{3+}_{0.38}Al_{0.62})_{\Sigma=4.97} \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.00} \ {}^{W}(F_{0.03}OH_{1.97})_{\Sigma=2.0$
160	member formula is ${}^{A}Na {}^{B}Na_{2} {}^{C}(Mg_{4}Al) {}^{T}Si_{8}O_{22} {}^{W}(OH)_{2}$, which requires SiO ₂ 59.80, Al ₂ O ₃ 6.34, MgO
161	20.05, Na ₂ O 11.57, H ₂ O 2.24, total 100.00 wt%.
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163	Compatibility
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165	The final $1 - (K_P/K_C)$ index for eckermannite AMNH H108401 is 0.010 (superior).
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167	Type material
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169	Type material for eckermannite is deposited in the collections of the Department of Earth and
170	Planetary Sciences, American Museum of Natural History, New York, New York, USA, specimen
171	number AMNH H108401. The refined and analyzed crystal of this work has the code 1213 in the
172	amphibole database of the CNR-IGG Pavia, where the refined fluoro-leakeite crystal from sample BM
173	1949.151 has the code 1161, and that from sample NMR 570725 has the code 1245.
174	
175	DISCUSSION
176	A comparison of the new holotype eckermannite from the Jade Mine tract, Myanmar, holotype
177	fluoro-leakeite from Norra Kärr, Sweden (Oberti et al., 2009), the former "holotype eckermannite" BM
178	1949.151, and the original material analyzed by Törnebohm (1906) (NMR 570725), is shown in Table
179	5. The three latter samples are nearly identical, both with regard to the geometrical (unit-cell
180	parameters and refined site geometry) and crystal-chemical (refined site-scattering values) parameters,
181	except for the higher site-scattering value refined at the $M(3)$ site in NMR 570725, which indicates a
182	slightly lower ^C Li content coupled with a slightly lower ${}^{M(2)}$ Fe ³⁺ content (as shown by the longer
183	< <i>M</i> (2)-O> distance). This confirms that samples BM 1949.151 and NMR 570725 are fluoro-leakeite,
184	and hence that eckermannite has never been found at Norra Kärr.
185	In contrast, eckermannite can be easily distinguished from fluoro-leakeite by comparing either
186	unit-cell parameters or optical properties or the details of the structure refinement.

187	Inspection of refined bond-lengths and site-scattering values allowed us to derive accurate site
188	populations starting from the unit formula obtained by EMP analysis. They are reported in Table 6. As
189	expected, trivalent cations are ordered at the $M(2)$ site. For comparison, the site populations derived for
190	the C cations in holotype fluoro-leakeite by Oberti et al. (2009) are: $M(1)$: 1.76 Mg + 0.20 Fe ²⁺ + 0.04
191	Zn, $d_{obs} = d_{cal} = 2.064$ Å; $M(2)$: 1.13 Al + 0.75 Fe ³⁺ + 0.09 Fe ²⁺ + 0.03 Ti ⁴⁺ , $d_{obs} = 1.968$ Å, $d_{cal} = 1.972$
192	Å; $M(3)$: 0.09 Mn ²⁺ + 0.91 Li ⁺ , $d_{obs} = 2.133$ Å, $d_{cal} = 2.105$ Å (which by the way implies that the effect
193	of ${}^{O(3)}F$ on the $M(3)$ site geometry in ^C Li amphiboles is lower than observed in "standard" amphiboles).
194	From the crystal-chemical point of view, the two amphibole compositions have the same charge
195	arrangement for the A, B, C, T groups of cations and W anions, but differ by: (i) the coupled
196	heterovalent exchange allowing the entrance of ^C Li into the amphibole structure, i.e. $M^{(2)}(Mg,Fe)^{2+}$ +
197	${}^{M(3)}(Mg,Fe)^{2+} \rightarrow {}^{M(2)}Fe^{3+} + {}^{M(3)}Li^+;$ (ii) the homovalent exchange ${}^{O(3)}(OH)^- \rightarrow {}^{O(3)}F^-$. Exchange (1)
198	makes the refined site-scattering value at $M(3)$ much lower and shortens the $< M(2)$ -O> distances
199	significantly, notwithstanding the fact that the Fe content in fluoro-leakeite is much higher (29.70 vs.
200	37.00 electrons per formula unit, epfu). Exchange (ii) shortens the $M(1,3)$ -O(3) distances significantly,
201	and hence the $< M(1,3)$ -O> distances; both these effects are evident from the structure refinements (note
202	that the $\langle M(3) - O \rangle$ distance is much larger in fluoro-leakeite due to the presence of Li ($\langle Li - O \rangle = 2.119$
203	Å and \langle Mg-O \rangle = 2.078 Å for amphiboles). Exchange (ii) also affects the ordering of A cations; as
204	expected (according to the conclusions of Hawthorne et al., 1996), Na occurs at the $A(m)$ and $A(2)$ sites
205	in eckermannite, but is ordered at $A(m)$ in fluoro-leakeite.
206	There are other issues which require comment: why are eckermannite compositions so rare in Nature,
207	and why are eckermannitic amphiboles often enriched in Fe (thus falling in the compositional field of
208	magnesio-arfvedsonite and arfvedsonite) or in fluorine? Hawthorne (1997) examined the effect of OH-
209	F substitution in arfvedsonite. In both arfvedsonite and fluoro-arfvedsonite, ^A Na is ordered at $A(m)$.
210	Where $M(2) = Mg$, the locally associated $A(m)$ site is occupied by Na. Where $M(2) = Al$, the locally
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211	associated $A(m)$ site is vacant; however, the A cavity still contains Na, but the Na occupies the $A(m)$ site
212	on the other side of the cavity, away from the $M(2)$ site containing Al. In arfvedsonite, the separation of
213	the two locally associated (split) $A(m)$ sites is quite small as the Na at $A(m)$ has to minimize its
214	interaction with the H atom of the OH group. In fluoro-arfvedsonite, the separation of the two locally
215	associated (split) $A(m)$ sites is considerably larger (Hawthorne et al. 1996, Fig. 8) as there is no H (i.e.
216	OH at the O(3) site) to repel Na. These interactions will be increased in eckermannite as the octahedral
217	strip contains Mg ₄ Al instead of $Fe^{2+}_{4}Fe^{3+}$ (as in arfvedsonite) and hence will be smaller, constraining
218	the A cavity to be smaller than in arfvedsonite and making the Na-H interaction in eckermannite even
219	more constraining than in arfvedsonite. These arguments suggest that arfvedsonite will be much more
220	common than eckermannite, and that the fluoro- species should be more common that the OH species.
221	
222	IMPLICATIONS
223	The results of this work emphasize that minerals with complex composition and crystal-
224	chemistry should be carefully characterized using a combination of independent techniques. In
225	particular, the occurrence of Li in amphiboles (either as a B or C cation, or both) should be carefully
226	checked where the geochemistry of the system is compatible with Li. The analyses reported by
227	Adamson (1942), but done by Törnebohm (1906), did not considered either F or Li; rather ironically,
228	the presence of Li would have been easier to detect at a time where wet-chemical analysis was the only
229	method to derive mineral composition. Indeed, Sundius (1945) reported the presence of Li in
230	amphiboles from Norra Kärr, but did not consider re-examination and possibly re-definition of
231	eckermannite. Admittedly, at this time, little was known about amphibole crystal-chemistry; however,
232	it is strong a that noith on A domagn non the other acientists studying the Norme Körn legality (a c
	it is strange that netwer Adamson hor the other scientists studying the Norra Karr locality (e.g.,
233	Adamson, 1944; von Eckermann, 1968; Blaxland, 1977; Kramm and Koark, 1988) re-considered the

235	refinement data of "eckermannite" would have quickly shown deficiencies in the chemical
236	characterization, confirming that SREF is a very powerful analytical technique.
237	Another conclusion to be drawn from the present work is that one must be cautious with regard
238	to the use of older names in amphiboles (and in other groups or supergroups of rock-forming minerals)
239	as names have been grandfathered without requiring proper characterization. Eckermannite and its
240	ferro- (i.e., magnesio-arfvedsonite) and fluoro-counterparts, katophorite and kaersutite, have all had
241	significant issues with regard to composition, and trivial names have been proposed after recognition
242	solely of homovalent substitutions. We hope that the latest report on amphibole nomenclature
243	(Hawthorne et al., 2012) has put some order in this matter and built a clear set of rules to be followed in
244	the future. In this regard, we are presently checking and characterizing some grandfathered
245	compositions
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247	ACKNOWLEDGMENTS
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 244 248 249 250 251 252 253 254 255 	Thanks are due to David Smith, loans manager of the Natural History Museum in London for providing a few crystals of sample BM 1949.151, and to Ulf Hålenius of the Swedish Museum of National History for providing crystals from the original material (NMR 570725) described by Törnebohm (1906). This work was funded by the MIUR grant 2009NHLC57_006 to the project "Structure, microstructures and cation ordering: a window on to geological processes and geomaterial properties" by R. Oberti, and by a Canada Research Chair in Crystallography and Mineralogy and a Discovery Grant to FCH from the Natural Sciences and Engineering Research Council of Canada, and
 244 248 249 250 251 252 253 254 255 256 	Thanks are due to David Smith, loans manager of the Natural History Museum in London for providing a few crystals of sample BM 1949.151, and to Ulf Hålenius of the Swedish Museum of National History for providing crystals from the original material (NMR 570725) described by Törnebohm (1906). This work was funded by the MIUR grant 2009NHLC57_006 to the project "Structure, microstructures and cation ordering: a window on to geological processes and geomaterial properties" by R. Oberti, and by a Canada Research Chair in Crystallography and Mineralogy and a Discovery Grant to FCH from the Natural Sciences and Engineering Research Council of Canada, and by Canada Foundation for Innovation grants to FCH
 247 248 249 250 251 252 253 254 255 256 257 	Thanks are due to David Smith, loans manager of the Natural History Museum in London for providing a few crystals of sample BM 1949.151, and to Ulf Hålenius of the Swedish Museum of National History for providing crystals from the original material (NMR 570725) described by Törnebohm (1906). This work was funded by the MIUR grant 2009NHLC57_006 to the project "Structure, microstructures and cation ordering: a window on to geological processes and geomaterial properties" by R. Oberti, and by a Canada Research Chair in Crystallography and Mineralogy and a Discovery Grant to FCH from the Natural Sciences and Engineering Research Council of Canada, and by Canada Foundation for Innovation grants to FCH

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- 317

- 318 **TABLE 1.** Refined site-scattering values (ss), atom coordinates and displacement parameters ($\beta_{ii} \times 10^4$)
- 319 for eckermannite AMNH H108401, fluoro-leakeite BM 1949.151(former eckermannite holotype) and
- 320 fluoro-leakeite NMR 570725.

Atom	ss (epfu.)	x/a	y/b	z/c	$B_{\rm eq}({\rm \AA}^2)$	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
AMNI	H H108401										
O(1)		0.11100(17)	0.08805(9)	0.21287(32)	0.85(3)	19	8	76	-2	9	-4
O(2)		0.11802(17)	0.16990(9)	0.73412(31)	0.94(4)	24	7	82	0	-4	-1
O(3)	16.49(6)	0.10828(24)	0	0.70978(46)	1.05(5)	25	9	101	-	7	-
O(4)		0.36274(19)	0.25079(10)	0.79757(34)	1.16(4)	43	7	103	-5	21	0
O(5)		0.34970(17)	0.12893(10)	0.08338(32)	1.03(4)	21	11	79	-1	3	8
O(6)		0.34156(17)	0.11827(10)	0.58486(32)	1.09(4)	27	11	73	0	4	-7
O(7)		0.33725(25)	0	0.28952(49)	1.15(6)	30	7	142	-	13	-
T(1)		0.27930(6)	0.08630(3)	0.29240(12)	0.67(1)	18	6	55	0	4	-1
T(2)		0.28706(6)	0.17250(3)	0.80083(12)	0.73(1)	21	6	59	-1	6	0
M(1)	25.72(14)	0	0.09002(6)	1/2	0.80(3)	23	7	66	-	8	-
M(2)	29.70(14)	0	0.18130(5)	0	0.81(2)	21	7	72	-	7	-
M(3)	12.95(4)	0	0	0	0.77(4)	24	6	58	-	4	-
M(4)	23.81(18)	0	0.27541(8)	¹ / ₂	1.51(4)	46	11	162	-	40	-
A	3.52(4)	0	1/2	0	1.6(2)	21	19	206	-	61	-
A(m)	3.03(11)	0.0259(16)	$\frac{1}{2}$	0.0717(25)	3.0(4)	80	26	245	-	10	-
A(2)	4.87(11)	0	0.4733(40)	0	3.1(2)	86	9	574	-	153	-
Н	1.75(16)	0.204(5)	0	0.740(9)	1.0						
BM 19	49.151										
O(1)		0.10796(9)	0.09295(5)	0.21081(17)	0.70(2)	15	7	64	-1	9	-2
O(2)		0.11774(9)	0.17108(5)	0.74128(18)	0.68(2)	16	6	70	0	8	1
O(3)	17.29(8)	0.11398(13)	0	0.69640(25)	0.99(3)	27	7	105	-	3	-
O(4)		0.36646(10)	0.25172(5)	0.80655(18)	0.80(2)	29	5	79	-4	20	-2
O(5)		0.35207(10)	0.12899(5)	0.08840(18)	0.73(2)	18	8	60	0	11	7
O(6)		0.34187(10)	0.12059(5)	0.58567(18)	0.76(2)	22	8	52	1	9	-7
O(7)		0.33211(15)	0	0.30121(28)	0.92(3)	30	4	115	-	14	-
T(1)		0.27745(3)	0.08705(2)	0.29475(7)	0.46(1)	14	4	41	-1	6	-1
T(2)		0.28951(3)	0.17255(2)	0.80684(6)	0.48(1)	15	4	40	-1	8	0
M(1)	28.83(8)	0	0.08757(3)	1/ ₂	0.59(1)	20	5	48	-	13	-
M(2)	36.50(8)	0	0.17914(2)	0	0.51(1)	15	4	48	-	8	-
M(3)	4.90(4)	0	0.0000	0	0.83(6)	27	5	76	-	2	-
M(4)	22.06(5)	0	0.27668(5)	1/ ₂	1.08(2)	37	7	121	-	40	-
Α	1.79(19)	0	1/2	0	1.5(1)						
A(m)	12.56(8)	0.0425(2)	1/2	0.0888(4)	2.7(1)	100	16	322	-	133	-
Н	0.49(10)	0.203(13)	0	0.734(24)	1.0						
NMR :	570725										
O(1)		0.10827(10)	0.09276(6)	0.21145(19)	0.82(2)	22	9	61	-1	10	-2
O(2)		0.11782(11)	0.17085(6)	0.74050(19)	0.81(2)	23	7	68	-1	7	0
O(3)	17.29(4)	0.11319(15)	0	0.69597(27)	1.10(3)	33	7	106	-	6	-
O(4)		0.36628(11)	0.25151(6)	0.80595(20)	0.98(2)	39	6	80	-4	21	0
O(5)		0.35170(11)	0.12899(6)	0.08874(19)	0.85(2)	24	9	60	0	11	7
O(6)		0.34210(11)	0.12043(6)	0.58625(19)	0.88(2)	27	9	57	0	10	-6
O(7)		0.33217(17)	0	0.30097(31)	1.10(3)	38	5	120	-	12	-
T(1)		0.27760(4)	0.08704(2)	0.29523(7)	0.59(1)	21	5	45	-1	8	-1
T(2)		0.28923(4)	0.17251(2)	0.80668(7)	0.62(1)	22	5	44	-1	10	0
M(1)	28.28(6)	0	0.08783(3)	1/2	0.72(1)	25	6	52	-	14	-
M(2)	36.63(5)	0	0.17940(2)	0	0.68(1)	22	6	53	-	11	-
M(3)	6.14(2)	0	0.0000	0	0.89(5)	31	6	72	-	9	-
				15							

<i>M</i> (4)	22.08(5)	0	0.27654(5)	1/2	1.25(2)	43	9	129	-	43	-
A	1.72(4)	0	1/2	0	1.4(2)	32	21	87	-	50	-
A(m)	12.72(8)	0.04191(35)	1/2	0.08706(65)	2.9(1)	111	17	340	-	138	-
Н	0.41(12)	0.208(5)	0	0.735(26)	1.0						

321

323 **TABLE 2**. Selected interatomic distances (Å) and angles (°) in eckermannite AMNH H108401 and

fluoro-leakeite BM 1949.151 and NMR 570725.

	AMNH	BM	NMR		AMNH	BM	NMR
	H108401	1949.151	570725		H108401	1949.151	570725
T(1)–O(1)	1.605(2)	1.600(1)	1.599(1)	T(2)–O(2)	1.612(2)	1.619(1)	1.616(1)
<i>T</i> (1)–O(5)	1.624(2)	1.628(1)	1.625(1)	T(2) - O(4)	1.584(2)	1.591(1)	1.588(1)
<i>T</i> (1)–O(6)	1.627(2)	1.626(1)	1.624(1)	<i>T</i> (2)–O(5)	1.668(2)	1.656(1)	1.657(1)
<i>T</i> (1)–O(7)	1.643(1)	1.630(1)	1.630(1)	<i>T</i> (2)–O(6)	1.678(2)	1.662(1)	1.662(1)
< <i>T</i> (1)–O>	1.625	1.621	1.619	< T(2)–O>	1.636	1.632	1.631
<i>M</i> (1)–O(1) ×2	2.068(2)	2.054(1)	2.052(1)	<i>M</i> (2)–O(1)×2	2.155(2)	2.027(1)	2.035(1)
<i>M</i> (1)–O(2) ×2	2.056(2)	2.102(1)	2.094(1)	<i>M</i> (2)–O(2) ×2	2.032(2)	1.988(1)	1.993(1)
<i>M</i> (1)–O(3) ×2	2.094(2)	2.039(1)	2.038(1)	<i>M</i> (2)–O(4) ×2	1.936(2)	1.894(1)	1.895(1)
< <i>M</i> (1)–O>	2.073	2.065	2.061	< <i>M</i> (2)–O>	2.041	1.970	1.974
<i>M</i> (3)–O(1) ×4	2.084(2)	2.119(1)	2.118(1)	<i>M</i> (4)–O(2) ×2	2.396(2)	2.394(1)	2.393(1)
<i>M</i> (3)–O(3) ×2	2.063(2)	2.159(1)	2.155(1)	<i>M</i> (4)–O(4) ×2	2.348(2)	2.362(1)	2.358(1)
< <i>M</i> (3)–O>	2.077	2.132	2.131	<i>M</i> (4)–O(5) ×2	2.900(2)	2.842(1)	2.842(1)
				<i>M</i> (4)–O(6) ×2	2.558(2)	2.493(1)	2.497(1)
<i>A</i> –O(5) ×4	2.823(2)	2.800(1)	2.802(1)	< <i>M</i> (4)–O>	2.551	2.523	2.523
<i>A</i> –O(6) ×4	3.175(2)	3.177(1)	3.172(2)				
<i>A</i> −O(7) ×2	2.460(3)	2.539(1)	2.537(2)	A(m)–O(5)×2	2.887(2)	2.941(2)	2.941(2)
<a-o></a-o>	2.891	2.899	2.897	A(m)–O(5)×2	2.816(2)	2.761(2)	2.761(2)
				A(m)–O(6) ×2	2.886(2)	2.803(2)	2.804(3)
A(2)–O(5) x2	2.450(2)	-	-	A(m)–O(7)	2.400(3)	2.558(2)	2.557(3)
A(2)–O(6) x2	2.880(2)	-	-	A(m)–O(7)	3.329(3)	3.158(2)	3.166(4)
A(2)–O(7) x2	2.505(3)	-	-	A(m)–O(7)	2.582(3)	2.636(2)	2.629(3)
< <i>A</i> (2)–O>	2.612			< <i>A</i> (<i>m</i>)–O>	2.832	2.818	2.818
O(3) –H	0.91(1)	0.84(1)	0.89(1)	<i>T</i> (1)–O(5)– <i>T</i> (2)	134.6(1)	133.6(1)	133.8(1)
M(1) - M(2)	3.107(1)	3.102(1)	3.100(1)	T(1) - O(6) - T(2)	137.9(1)	139.0(1)	138.7(1)
() -(-)	(-)	(-)	(-)	T(1)-O(7)-T(1)	139.2(1)	142.5(1)	142.5(1)
O(5)–O(6)–O(5)	171.1(1)	172.3(1)	172.4(1)	O(6)–O(7)–O(6)	107.3(1)	110.5(1)	110.3(1)

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324

Irel	d(calc)	h k l	Irel	d(calc)	h k l	Irel	d(calc)	h k l	$I_{\rm rel}$	d(calc)	h k l
4	8.920	0 2 0	36	2.574	061	4	1.921	-3 5 2	8	1.628	4 8 0
42	8.407	1 1 0			0 0 2	9	1.895	5 1 0	9	1.599	1 1 1 0
13	4.859	-1 1 1	56	2.525	-202	4	1.876	2 4 2	6	1.588	600
6	4.766	$2 \ 0 \ 0$	5	2.384	-2 6 1	4	1.862	-4 6 1	21	1.579	-1 5 3
30	4.460	040	7	2.373	3 5 0	8	1.846	-191	11	1.521	-6 0 2
9	4.028	1 1 1	27	2.315	-3 5 1	4	1.824	-4 4 2	23	1.508	-2 6 3
16	3.850	-1 3 1	18	2.275	-171	4	1.816	530	14	1.487	0 12 0
59	3.395	131	20	2.261	-3 1 2	7	1.786	191	6	1.445	3 11 0
34	3.257	240	9	2.197	-2 4 2			0 10 0	6	1.440	-6 4 2
56	3.128	310	33	2.161	261	4	1.732	-5 1 2	28	1.430	-661
7	2.997	-3 1 1	10	2.128	-3 3 2	9	1.687	-1 3 3	3	1.415	-533
33	2.966	060	17	2.067	2 0 2			0 2 3	11	1.379	5 1 2
12	2.915	-1 5 1	9	2.023	3 5 1	9	1.684	-1 3 3	7	1.348	-553
18	2.802	3 3 0	8	1.999	-4 0 2			0 2 3			532
100	2.702	-331	6	1.942	4 2 1	8	1.672	-2 8 2			
		1 5 1			190	25	1.654	4 6 1			

327 **TABLE 3.** Powder X-ray data for eckermannite AMNH H108401. The ten strongest line are in bold.

- 329 **TABLE 4.** EMP analysis (10 points) and unit formula calculated based on 24 (O,OH,F,Cl) and 2
- 330 (OH,F,Cl) for the refined crystal of holotype eckermannite AMNH H108401 (1213 in the CNR-IGG-
- 331 Pv database); ss = site scattering (electrons per formula unit, epfu); bdl = below detection limit

	wt%	esd		apfu			
SiO ₂	59.30	0.24	Si	8.00			
TiO ₂	0.03	0.02	Al	0.00			
Al_2O_3	3.89	0.61	ΣΤ	8.00			
Cr_2O_3	bdl		Ti	0.00			
Fe ₂ O ₃	3.78		Al	0.62			
FeO*	0.80		Fe ³⁺	0.38			
MnO	0.07	0.02	Fe^{2+}	0.09			
MgO	19.25	0.14	Mg	3.87			
ZnO	bdl		Mn^{2+}	0.01			
CaO	0.77	0.12	ΣC	4.97			
Na ₂ O	10.56	0.18	Ca	0.11			
K_2O	0.32	0.03	Na	1.89			
F	0.06	0.04	ΣΒ	2.00			
Cl	bdl		Na	0.87			
O=F,Cl	0.03		Κ	0.06			
$(H_2O)_{cal}$	2.19		ΣΑ	0.93			
			F	0.03			
Total	101.00		OH	1.97			
			ΣW	2.00			
calculate	d ss		refined	l ss			
ss (67.08		ss C	68 37			
ss B	23.00		ss B	23.81			
ss A	10.35		ss A	11 42			
Total	100.75		Total	103.60			
* esd for FeO(total) = 0.59							

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10/29

334 TABLE 5. Comparative data for holotype eckermannite AMNH H108401 (this work), holotype fluoro-

leakeite (Oberti et al., 2009), the discredited holotype eckermannite kept at the Natural History

336 Museum in London (with optical properties taken by the compilation in the Handbook of Mineralogy

337 (Anthony et al., presently \mathbb{C} MSA) and marked with *), and sample NMR 570725 originally described

338 in Törnebohm (1906).

	Eckermannite Jade Mine tract AMNH H10840	Fluoro-leakeite Norra Kärr 1	e "Eckermannite" Norra Kärr BM 1949.151	"Eckermannite" Norra Kärr NMR 570725
a (Å)	9.8087(7)	9.7043(5)	9.7073(5)	9.7094(6)
b	17.8448(13)	17.7341(8)	17.7339(6)	17.7305(12)
с	5.2905(4)	5.2833(3)	5.2850(4)	5.2815(3)
β (°)	103.660(1)	104.067(4)	104.029(5)	104.040(1)
$V(Å^3)$	899.83(11)	881.97(8)	882.67(9)	882.06(10)
a:b:c	0.550:1:0.297	0.547:1:0.298	0.547:1:0.298	0.548:1:0.298
Space group	<i>C</i> 2/ <i>m</i>	C2/m	<i>C</i> 2/ <i>m</i>	<i>C</i> 2/ <i>m</i>
Optic sign	Biaxial (-)	Biaxial (-)	Biaxial (-)*	Biaxial (-)
α	1.605	1.632	1.610-1.640*	1.636
β	1.630	1.638	1.625-1.650*	1.644
γ	1.634	1.643	1.630-1.655*	1.649
2 <i>V</i> (°)	43	98	15-80*	74
Colour	Pale grey	Pale greenish blue	Bluish green to dark green*	Bluish green to dark green*
Pleochroism	Pale grey to	Pale-green to	Pale green to	Colourless to
	medium grey	dark-green	dark green	bluish green
< T(1)-O>(Å)	1.625	1.620	1.621	1.619
< T(2)-O>(Å)	1.636	1.631	1.632	1.631
< <i>M</i> (1)-O>(Å)	2.073	2.064	2.065	2.061
< M(2)-O>(Å)	2.041	1.968	1.970	1.974
< <i>M</i> (3)-O>(Å)	2.077	2.133	2.132	2.131
< M(4)-O>(Å)	2.551	2.523	2.523	2.523
ss $M(1)$ (epfu)	25.72	28.86	28.83	28.28
ss $M(2)$ (epfu)	29.70	37.00	36.50	36.63
ss $M(3)$ (epfu)	12.95	4.81	4.90	6.14
ss $M(4)$ (epfu)	23.81	22.30	22.06	22.08
ss A (epfu)	3.52	3.75	1.79	1.72
ss $A(m)$ (epfu)	3.03	10.69	12.56	12.72
ss $A(2)$ (epfu)	4.87	-	-	-

339 **TABLE 6.** Site occupancies proposed for eckermannite AMNH H108401 based on the results of

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the structure refinement.

Site	Site nonvolution (antra)	site scattering (epfu)				
Site	Site population (apru)	refined	calculated			
<i>T</i> (1)	4 Si					
<i>T</i> (2)	4 Si					
<i>M</i> (1)	$1.90 \text{ Mg} + 0.10 \text{ Fe}^{2+}$	25.72	25.40			
<i>M</i> (2)	$1.04 \text{ Mg} + 0.62 \text{ Al} + 0.34 \text{ Fe}^{3+}$	29.70	29.38			
<i>M</i> (3)	0.96 Mg + 0.03 Fe ²⁺ + 0.01 Mn	12.95	12.55			
ΣC sites	-	69.37	67.33			
B site	1.89 Na + 0.11 Ca	23.81	22.99			
A site	0.87 Na + 0.06 K	11.42	10.71			

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- 346 FIGURE 1. Jadeitite-amphibole fels rock catalogued as AMNH H108401 in the mineral collection of the
- 347 American Museum of Natural History

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