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Magnesio-hornblende from Lüderitz, Namibia: mineral description and crystal chemistry

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ABSTRACT

Magnesio-hornblende (IMA2017-059) has been characterized in a specimen collected in the sand dunes of Lüderitz, Karas Region, Namibia. The empirical formula derived from electron microprobe analysis and single-crystal structure refinement is $^{A}(\square_{0.73}Na_{0.22}K_{0.05})_{\Sigma 1.00}{}^{B}(Ca_{1.79}Fe^{2+}_{0.10}Mg_{0.04}Mn^{2+}_{0.03}Na_{0.04})_{\Sigma 2.00}$ $^{C}(Mg_{3.48}Fe^{2+}_{0.97}Al_{0.28}Fe^{3+}_{0.23}Cr^{3+}_{0.01}Ti_{0.03})_{\Sigma 5.00}{}^{T}(Si_{7.18}Al_{0.82})_{\Sigma 8.00}O_{22}{}^{W}[(OH)_{1.93}F_{0.05}Cl_{0.02}]_{\Sigma 2.00}$. Magnesio-hornblende is biaxial (–), with $\alpha = 1.640(2)$, $\beta = 1.654(2)$, $\gamma = 1.666(2)$ (measured with gel-filtered Na light, $\lambda = 589.9$ nm), 2V (meas.) = 82(1)° and 2V (calc.) = 84.9°. The unit-cell parameters are $a = 9.8308(7)$, $b = 18.0659(11)$, $c = 5.2968(4)$ Å, $\beta = 104.771(6)°$ and $V = 909.64$ (11) Å^3 with $Z = 2$ and space group *C*2/*m*. The strongest eight reflections in the X-ray powder pattern [*d* values (in Å), *I*, (*hkl*)] are: 2.709, 100, (151); 8.412, 74, (110); 3.121, 73, (310); 2.541, 58, ($\bar{2}$02); 3.386, 49, (131); 2.596, 45, (061); 2.338, 41, ($\bar{3}$51); and 2.164, 39, (261).

Keywords: magnesio-hornblende, electron-microprobe analysis, optical properties, powder-diffraction pattern, crystal-structure refinement, Lüderitz, Namibia.

Introduction

The generic name 'hornblende' is used widely by petrologists and mineral collectors for any black undefined Al-bearing amphibole in the calcium (and sometimes in the sodium–calcium) subgroups. Therefore, the currently approved scheme for amphibole nomenclature and classification (Hawthorne *et al*., 2012) uses the rootname hornblende for the charge arrangement $^{A}\square^{B}Ca_2{}^{C}(R^{2+}_4R^{3+})^{T}(Si_7Al)O_{22}{}^{W}(OH,F,Cl)_2$ where Al is dominant over R^{3+} cations and the prefix 'magnesio-' indicates Mg dominance over R^{2+} cations (exceptions are allowed only for riebeckite, arfvedsonite, hastingsite and hornblende).

Despite its widespread occurrence (~220 compositions listed in the mindat.org web page: https://www.mindat.org/min-2524.html, some of which should not be classified as magnesio-hornblende), the type description of an amphibole with composition corresponding to $^{A}\square^{B}Ca_2{}^{C}(Mg_4Al)^{T}(Si_7Al)O_{22}{}^{W}(OH)_2$ has never been published.

In the most recent list of minerals approved by the International Mineralogical Association (IMA version July 2017; https://www.ima-mineralogy.org/Minlist.htm), magnesio-hornblende is designated as a redefined valid species (by Hawthorne *et al*., 2012) with unknown type locality and without an original reference. Therefore, it is a potential new species which requires formal approval by the IMA Commission on New Minerals, Nomenclature and Classification (CNMNC) and publication of the mineral data. This work describes magnesio-hornblende from Lüderitz, Namibia approved by IMA-CNMNC vote 2017-059.

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Occurrence and optical properties

The specimen under investigation was found in 1970 by MEC in the sand dunes of the Lüderitz, Karas Region, Namibia (~26°38′52″S, 15°09′28″E). Lüderitz is a surreal colonial relic, a true 19th century Bavarian village at the southern margin of the Namib Desert coast. It was founded in 1883 as a trading post, and in 1909 enjoyed a sudden but short period of prosperity when diamonds were discovered nearby. The Namib Desert was part of the passive margin during Early Cretaceous rifting of the South Atlantic, and extends for nearly 600 km along the Namibian coast between Lüderitz (~27°S) and the Kuiseb River (~23°S); it is 100 to 150 km wide, extending inland from the coast to the base of the Great Escarpment at the 1000 m contour. The sand sea (~34,000 km^2) is dominated by large linear dunes, with areas of star-shaped dunes on its eastern margin and a belt of simple and compound transverse and barchanoid dunes (Fig. 1) along the coast (Garzanti *et al.*, 2012). Dune sands in the coastal Namib are invariably lithofeldspatho–quartzose volcaniclastic, and have a homogeneous composition from Lüderitz to Walvis Bay. They were originally deposited by the Orange River, which has its source 3000 km away in the basaltic rift highlands of Lesotho and flows into the ocean 300 km south of Lüderitz, to which sands are dragged by vigorous longshore currents (Garzanti *et al.*, 2012). Plagioclase exceeds K-feldspar. In the sand, mafic volcanic rock fragments predominate over granitoid, sedimentary (quartzose to feldspatho–quartzose siltstone/sandstone, shale, minor limestone and hybrid carbonate) and metamorphic (quartz–sericite, quartz–mica, quartz–epidote, amphibolite) grains. Samples enriched in heavy minerals are usually dominated by clinopyroxene, with subordinate opaque Fe–Ti–Cr oxides, garnet, epidote and amphibole. Landward of Lüderitz, the quartz content increases at the expense of volcanic detritus; garnet, Fe–Ti–Cr oxides, amphibole (including green and green-brown hornblende), epidote, titanite, staurolite and zircon also become more significant, suggesting contributions from the Koichab River and the locally exposed Namaqua basement rocks (Garzanti *et al.*, 2012).

The holotype specimen (Fig. 2) consists of a friable block of subhedral to anhedral magnesio-hornblende crystals up to a few mm in size. The crystals are green to dark green with good cleavage parallel to {110}. A spindle stage was used to orient a crystal for measurement of refractive indices and 2V by extinction curves (Bartelmehs *et al.*, 1992). The optical orientation was determined by transferring the crystal from the spindle stage to a single-crystal diffractometer and measuring the relative axial relations by X-ray diffraction. In transmitted plane-polarized light, magnesio-hornblende is pleochroic (X = pale yellow, Y = bluish green, Z = dark green) with $Z > Y > X$. Magnesio-hornblende is non fluorescent and has a vitreous lustre. It is biaxial (–), with $\alpha = 1.640(2)$, $\beta = 1.654(2)$, $\gamma = 1.666(2)$ (measured with gel-filtered Na light, $\lambda = 589.9$ nm), 2V (meas.) = 82(1)° and 2V (calc.) = 84.9°. The dispersion is weak ($v > r$), and the orientation is: $X \wedge a = 33.7°$ (in β obtuse), $Y \parallel b$, $Z \wedge c = 18.2°$ (in β acute). The density calculated based on the chemical formula and the unit-cell parameters is 3.137 g·cm^{-3}. The compatibility index $[1 - (K_p/K_c)]$ (Mandarino, 2007) is 0.010 (superior).

The holotype material is deposited in the mineralogical collections of the Museo di Mineralogia, Sistema Museale di Ateneo,

FIG. 1. Barchanoid dunes near Lüderitz.

FIG. 2. The holotype specimen studied in this work. Scale in cm.

TABLE 1. Atom coordinates, refined site-scattering values* (ss, epfu), and equivalent atom-displacement parameters (B_{eq}, Å^2) for magnesio-hornblende crystal 1325.

Site	ss	*x/a*	*y/b*	*z/c*	B_{eq}
O(1)		0.1090(2)	0.08794(11)	0.2154(4)	0.76(4)
O(2)		0.1194(2)	0.17303(10)	0.7295(4)	0.70(4)
O(3)	16.04(12)	0.1108(3)	0	0.7149(5)	0.81(7)
O(4)		0.3680(2)	0.24863(11)	0.7904(4)	0.94(4)
O(5)		0.3482(2)	0.13658(11)	0.1022(4)	0.95(4)
O(6)		0.3435(2)	0.11837(11)	0.5944(4)	0.93(4)
O(7)		0.3361(3)	0	0.2858(6)	1.06(6)
T(1)		0.28034(7)	0.08481(4)	0.29774(14)	0.45(2)
T(2)		0.29007(7)	0.17183(4)	0.80727(13)	0.51(2)
M(1)	31.56(14)	0	0.08892(5)	½	0.61(2)
M(2)	29.73(14)	0	0.17739(5)	0	0.52(2)
M(3)	16.40(6)	0	0	0	0.57(3)
M(4)	37.8(2)	0	0.27851(5)	½	0.77(2)
M(4’)	2.34(10)	0	0.2549(10)	½	1.0
A	0.89(8)	0	½	0	2.0
A(*m*)	0.84(11)	0.028(6)	½	0.081(14)	2.0
A(2)	1.67(11)	0	0.478(2)	0	2.0
H	1.96	0.196(6)	0	0.758(10)	1.0

*Hawthorne *et al.* (1995); ‘epfu’ – electrons per formula unit.

TABLE 2. Selected interatomic distances (Å), angles (°), tetrahedral and octahedral angle variances (TAV, OAV, °^2) and quadratic elongations (TQE, OQE) according to Robinson *et al.* (1971) refined for magnesio-hornblende crystal 1325.

T(1)–O(1)	1.630(2)	*T*(2)–O(2)	1.623(2)	*M*(4)–O(2) ×2	2.400(2)
T(1)–O(5)	1.657(2)	*T*(2)–O(4)	1.598(2)	*M*(4)–O(4) ×2	2.304(2)
T(1)–O(6)	1.651(2)	*T*(2)–O(5)	1.648(2)	*M*(4)–O(5) ×2	2.723(2)
T(1)–O(7)	1.6337(12)	*T*(2)–O(6)	1.668(2)	*M*(4)–O(6) ×2	2.545(2)
<*T*(1)–O>	1.643	<T(2)–O>	1.634	<*M*(4)–O>	2.493
TAV	4.40	TAV	19.50		
TQE	1.0010	TQE	1.0049		
M(1)–O(1) ×2	2.060(2)	*M*(2)–O(1) ×2	2.107(2)	*M*(3)–O(1) ×4	2.086(2)
M(1)–O(2) ×2	2.106(2)	*M*(2)–O(2) ×2	2.072(2)	*M*(3)–O(3) ×2	2.075(3)
M(1)–O(3) ×2	2.105(2)	*M*(2)–O(4) ×2	1.992(2)	<*M*(3)–O>	2.082
<*M*(1)–O>	2.090	<*M*(2)–O>	2.057	OAV	58.09
OAV	40.78	OAV	22.51	OQE	1.0180
OQE	1.0126	OQE	1.0072		
A–O(5) ×4	3.003(2)	*A*(*m*)–O(5) ×2	3.05(3)	*A*(2)–O(5) ×2	2.69(3)
A–O(6) ×4	3.142(2)	*A*(*m*)–O(5) ×2	3.02(3)	*A*(2)–O(6) ×2	2.89(2)
A–O(7) ×2	2.477(3)	*A*(*m*)–O(6) ×2	2.83(5)	*A*(2)–O(7) ×2	2.507(6)
<*A*–O>	2.953	*A*(*m*)–O(7)	2.40(5)	<*A*(2)–O>	2.70
		A(*m*)–O(7)	3.28(7)		
M(4’)–O(2) ×2	2.077(13)	*A*(*m*)–O(7)	2.63(6)	*T*(1)–O(5)–*T*(2)	135.48(12)
M(4’)–O(4) ×2	2.253(2)	<*A*(*m*)–O>	2.90	*T*(1)–O(6)–*T*(2)	138.52(12)
M(4’)–O(5) ×2	2.985(12)			*T*(1)–O(7)–*T*(1)	139.4(2)
M(4’)–O(6) ×2	2.872(14)	*M*(1)–*M*(2)	3.213(2)	O(5)–O(6)–O(5)	165.71(12)
<*M*(4’)–O>	2.547			O(6)–O(7)–O(6)	105.81(13)

TABLE 3. Powder X-ray diffraction data (*d* in Å) for magnesio-hornblende crystal 1325.

I_{rel}	*d*(calc)	*h k l*	I_{rel}	*d*(calc)	*h k l*
22.9	9.033	0 2 0	**39.2**	**2.164**	**2 6 1**
74.2	**8.412**	**1 1 0**	5.4	2.137	$\bar{1}$ 5 2
8.7	5.088	1 3 0	20.0	2.047	2 0 2
22.3	4.892	$\bar{1}$ 1 1	27.5	2.017	3 5 1
16.2	4.516	0 4 0			$\bar{4}$ 0 2
5.3	4.206	2 2 0	8.4	2.002	3 7 0
16.4	3.884	$\bar{1}$ 3 1	5.2	1.965	1 9 0
48.5	**3.386**	**1 3 1**	6.3	1.890	5 1 0
29.1	3.274	2 4 0	5.8	1.877	$\bar{4}$ 6 1
72.5	**3.121**	**3 1 0**	11.7	1.867	$\bar{1}$ 9 1
33.9	2.941	2 2 1	5.6	1.848	$\bar{1}$ 7 2
11.5	2.804	3 3 0	5.0	1.843	$\bar{4}$ 4 2
31.0	2.731	$\bar{3}$ 3 1	5.0	1.812	5 3 0
100.0	**2.709**	**1 5 1**	5.9	1.747	$\bar{5}$ 1 2
45.4	**2.596**	**0 6 1**	13.6	1.689	$\bar{1}$ 3 3
57.5	**2.541**	**$\bar{2}$ 0 2**			$\bar{2}$ 8 2
8.4	2.382	3 5 0	8.2	1.678	0 2 3
40.7	**2.338**	**$\bar{3}$ 5 1**	26.7	1.650	4 6 1
20.3	2.322	$\bar{4}$ 2 1	8.1	1.637	4 8 0
14.8	2.301	$\bar{1}$ 7 1	12.4	1.618	1 11 0
20.7	2.280	$\bar{3}$ 1 2	28.1	1.583	6 0 0
7.8	2.215	$\bar{2}$ 4 2			$\bar{1}$ 5 3
7.9	2.182	1 7 1	6.9	1.556	4 0 2

The strongest eight reflections are in bold. Only peaks with $I_{rel} \geq 5$ are reported.

University of Pavia, under the catalogue number 2017-01. The refined and analysed crystal of this work has the code 1325 in the amphibole database of the CNR-IGG Pavia.

Single-crystal diffraction and powder-diffraction analysis

The crystal studied is 0.60 mm × 0.45 mm × 0.10 mm in size. The unit-cell parameters are $a = 9.8308(7)$, $b = 18.0659(11)$, $c = 5.2968(4)$ Å, $\beta = 104.771(6)°$ and $V = 909.64$ (11) Å^3, and were calculated by a least-squares procedure using the *d** values measured for reflections belonging to 60 selected rows of reciprocal space and occurring in the θ range –30° to + 30°. Two monoclinic equivalents were collected in the 2θ range 4–60° by a Philips PW1100 4-circle diffractometer using Mo*K*α radiation; absorption and Lorentz and polarization corrections were applied. Merging of equivalent reflections gave $R_{sym} = 2.60\%$ on 1290 pairs. Reflections with $I > 3\sigma_I$ were considered as observed during unweighted full-matrix least-squares refinement on *F* using a program locally written to deal with complex solid-solutions (Cannillo *et al.*, 1983). Scattering curves for fully ionized chemical species were used at sites where chemical substitutions occur; neutral *vs.* ionized scattering curves were used at the *T* and at the anion sites [except O(3)]. More details on the refinement strategy can be found in Oberti *et al.* (1992) and Oberti *et al.* (2017). The final disagreement indexes are $R_{obs} = 2.72\%$ (1244 reflections) and $R_{all} = 3.15\%$ (1380 reflections). Refined atom coordinates and displacement parameters, and selected bond lengths and angles are given in Tables 1 and 2, respectively. Crystallographic information files with embedded structure factors have been deposited with the Principal Editors of *Mineralogical Magazine* and are available as supplementary material (see below). The *a*:*b*:*c* ratio calculated from the unit-cell parameters is 0.544:1:0.293.

Powder X-ray diffraction data (Cu*K*α, λ = 1.54178 Å) were obtained using the *XPREP* utility of *SAINT* (Bruker, 2003), which generates a 2D powder diffractogram (Debye-Scherrer technique) starting from the F^2_{obs} collected on the single crystal and taking into account solely the information concerning the unit-cell dimensions and the Laue symmetry. No Lorentz and polarization corrections were applied. Data are given in Table 3.

Chemical analysis

Chemical analysis (10 points) on the crystal used for structure refinement was undertaken with a Cameca SX-100 electron microprobe (WDS mode, 15 kV, 20 nA, count time 20 s and 5 µm beam diameter). The standards used are as follows: Si and Ca: diopside (TAP); Ti: titanite (LPET); Al: andalusite (TAP); Cr: chromite (LPET); Fe: fayalite (LLiF); Mn: spessartine (LLiF); Mg: forsterite (LTAP); Zn: gahnite (LLiF); Ni: pentlandite (LLiF); Na: albite (TAP); K: orthoclase (LPET); F: fluoro-riebeckite (TAP) and Cl: tugtupite (LPET). H_2O was estimated based on 2 = (OH,F,Cl) atoms per formula unit (apfu) and taking into account the constraints on the group sites based on stoichiometry and site-scattering values (for A, B and C cations) obtained from the structure refinement; this method allows calculation of Fe^{3+}/Fe^{2+}. The oxide wt.% and the calculated unit-formula are reported in Table 4. The proposed empirical formula for crystal 1325 is: $^{A}(\square_{\mathbf{0.73}}Na_{0.22}K_{0.05})_{\Sigma 1.00}\,^{B}(\mathbf{Ca}_{\mathbf{1.79}}Fe^{2+}_{0.10}Mg_{0.04}Mn^{2+}_{0.03}Na_{0.04})_{\Sigma 2.00}\,^{C}(\mathbf{Mg}_{\mathbf{3.48}}Fe^{2+}_{0.97}Al_{0.28}Fe^{3+}_{0.23}Cr^{3+}_{0.01}Ti_{0.03})_{\Sigma 5.00}\,^{T}(Si_{7.18}Al_{0.82})_{\Sigma 8.00}O_{22}\,^{W}[\mathbf{(OH)}_{\mathbf{1.93}}F_{0.05}$

TABLE 4. Chemical composition (10 analytical points), unit formula (based on 24 anions and 15.27 cations) and a comparison between observed and calculated site scattering for magnesio-hornblende (1325).

Oxide	Wt.%(esd)	Range	Apfu			
SiO_2	50.24(23)	49.16–51.10	Si	7.18	Ca	1.79
TiO_2	0.24(2)	0.22–0.25	Al	0.82	Na	0.04
Al_2O_3	6.52(7)	6.26–6.72	Sum T	8.00	Fe^{2+}	0.10
Fe_2O_3	2.17				Mn^{2+}	0.03
Cr_2O_3	0.10(2)	0.08–0.11	Ti^{4+}	0.03	Mg	0.04
V_2O_3	0.03(4)	0.00–0.05	Al^{3+}	0.28	Sum B	2.00
FeO	8.87		Fe^{3+}	0.23		
$[FeO]_{tot}$	[10.82(20)]	10.69–10.98	V^{3+}	–	Na	0.22
MgO	16.52(9)	16.44–16.59	Cr^{3+}	0.01	K	0.05
MnO	0.25(5)	0.23–0.28	Mg	3.48	Sum A	0.27
NiO	0.03(5)	0.00–0.06	Mn^{2+}	–		
ZnO	0.02(6)	0.00–0.07	Fe^{2+}	0.97	$(OH)^-$	1.93
CaO	11.68(12)	11.64–11.75	Ni	–	F^-	0.05
Na_2O	0.92(6)	0.87–1.01	Zn	–	Cl	0.02
K_2O	0.30(2)	0.23–0.35	Sum C	5.00	Sum W	2.00
H_2O*	2.02			Group site scattering (epfu)		
F	0.11(30)	0.00–0.31		obs (SREF)		calc (EMP)
Cl	0.10		C	77.69		77.50
O = F	−0.05		B	40.14		40.07
O = Cl	−0.02		A	3.40		3.37
Total	100.05		Total	121.23		120.94

* calculated based on 24 (O, OH, F, Cl) with (OH + F + Cl) = 2 apfu.

TABLE 5. Site populations for magnesio-hornblende, crystal 1325. There is close agreement between the refined values of site-scattering (ss, epfu) and mean bond lengths (mbl, Å) and those calculated based on the proposed site-populations*.

Site	Site population (apfu)	ss (epfu)		mbl (Å)	
		Refined	Calc.	Refined	Calc.
T(1)	3.18 Si + 0.82 Al			1.643	1.643
T(2)	4.00 Si			1.634	
M(1)	1.46 Mg + 0.54 Fe^{2+}	31.56	31.56	2.090	2.090
M(2)	1.37 Mg + 0.14 Fe^{2+}+ 0.22 Al + 0.23 Fe^{3+} + 0.01 Cr^{3+}+ 0.03 Ti^{4+}	29.73	29.82	2.057	2.056
M(3)	0.65 Mg + 0.29 Fe^{2+} + 0.06 Al	16.40	16.12	2.082	2.082
ΣC cations		77.69	77.50		
B cations	1.79 Ca + 0.10 Fe^{2+} + 0.03 Mn^{2+}+ 0.04 Mg + 0.04 Na	40.14	40.07		
A cations	0.22 Na + 0.05 K	3.40	3.37		
W anions	1.93 $(OH)^-$ + 0.05 F^- + 0.02 Cl^-	16.04	16.23		

*Hawthorne *et al.* (1995)

$Cl_{0.02}]_{\Sigma 2.00}$ (where the dominant cations/anions relevant to nomenclature issues are in bold). The simplified end-member formula of magnesio-hornblende is $^{A}\square^{B}Ca_2{}^{C}(Mg_4Al)^{T}(Si_7Al)O_{22}{}^{W}(OH)_2$, which requires SiO_2 51.68, Al_2O_3 12.53, MgO 19.80, CaO 13.78, H_2O 2.21, total 100.00 wt.%.

TABLE 6. A comparison of the optical and crystallographic properties available for magnesio-hornblende (this work), magnesio-ferri-fluoro-hornblende (Oberti *et al*., 2016*a*), and ferro-ferri-hornblende (Oberti *et al*., 2016*b*).

	Magnesio-hornblende[1]	Magnesio-ferri-fluoro-hornblende[2]	Ferro-ferri-hornblende[3]
Colour	Dark green	Dark brown	Dark green
Optical class	Biaxial (–)	Biaxial (–)	Biaxial (–)
Pleochroism	X = pale yellow	X = pale grey	X = medium gold/brown
	Y = bluish green	Y = dark grey	Y = dark brown/black
	Z = dark green	Z = pale brownish grey	Z = dark grey
Orientation	$X \wedge a$ = 33.7° (β obtuse)	$X \wedge a$ = 47.6° (β obtuse)	$X \wedge a$ = 26.2° (β obtuse)
	$Y \parallel b$	$Y \parallel b$	$Y \parallel b$
	$Z \wedge c$ = 18.2° (β acute)	$Z \wedge c$ = 33.4° (β acute)	$Z \wedge c$ = 11.5° (β acute)
α	1.640(2)	1.669(2)	1.697(2)
β	1.654(2)	1.676(2)	1.722(5)
γ	1.666(2)	1.678(2)	1.726(5)
$2V_{meas}$ (°)	85(1)°	74(1)°	35.7(4)°
Space group	*C*2/*m*	*C*2/*m*	*C*2/*m*
a (Å)	9.8308(7)	9.839(5)	9.9307(5)
b (Å)	18.0659(11)	18.078(9)	18.2232(10)
c (Å)	5.2968(4)	5.319(3)	5.3190(3)
β (°)	104.771(6)	104.99(3)	104.857(1)
V (Å^3)	909.64(11)	913.9(9)	930.40(9)
<*T*(1)–O> (Å)	1.643	1.642	1.642
<*T*(2)–O> (Å)	1.634	1.636	1.635
<*M*(1)–O> (Å)	2.090	2.078	2.117
<*M*(2)–O> (Å)	2.057	2.067	2.086
<*M*(3)–O> (Å)	2.082	2.076	2.111
<*M*(4)–O> (Å)	2.493	2.502	2.514
T(1)–O(5)–*T*(2) (°)	135.5	136.4	136.7
T(1)–O(6)–*T*(2) (°)	138.5	139.8	139.1
T(1)–O(7)–*T*(1) (°)	139.4	140.0	141.3
O(5)–O(6)–O(5) (°)	165.7	167.6	167.8
O(6)–O(7)–O(6) (°)	105.8	108.5	108.3

[1] $^{A}(\square_{0.73}Na_{0.22}K_{0.05})_{\Sigma1.00}{}^{B}(Ca_{1.79}Fe^{2+}_{0.10}Mn^{2+}_{0.03}Mg_{0.04}Na_{0.04})_{\Sigma2.00}{}^{C}(Mg_{3.48}Fe^{2+}_{0.97}Al_{0.28}Fe^{3+}_{0.23}Cr^{3+}_{0.01}Ti_{0.03})_{\Sigma5.00}$ $^{T}(Si_{7.18}Al_{0.82})_{\Sigma8.00}O_{22}{}^{W}[(OH)_{1.93}F_{0.05}Cl_{0.02}]_{\Sigma2.00}$

[2] $^{A}(\square_{0.63}Na_{0.15}K_{0.22})_{\Sigma1.00}{}^{B}(Ca_{1.66}Mn_{0.09}Na_{0.25})_{\Sigma1.00}{}^{C}(Mg_{2.20}Fe^{2+}_{1.94}Mn_{0.01}Zn_{0.01}Fe^{3+}_{0.72}Ti_{0.13})_{\Sigma5.01}$ $^{T}(Si_{6.89}Al_{1.11})_{\Sigma8.00}O_{22}{}^{W}[F_{1.55}(OH)_{0.37}Cl_{0.08})_{\Sigma2.00}$

[3] $^{A}(\square_{0.77}Na_{0.10}K_{0.13})_{\Sigma1.00}{}^{B}(Ca_{1.93}Na_{0.07})_{\Sigma2.00}{}^{C}(Mg_{1.16}Fe^{2+}_{3.21}Mn_{0.06}Fe^{3+}_{0.45}Al_{0.12}Ti_{0.01})_{\Sigma5.01}$ $^{T}(Si_{7.26}Al_{0.74})_{\Sigma8.00}O_{22}{}^{W}(OH_{1.89}F_{0.01}Cl_{0.10})_{\Sigma2.00}$

The crystal chemistry of magnesio-hornblende

Site populations were obtained taking into account the experimental mean bond lengths and site-scattering values for the individual sites (Hawthorne *et al*., 1995; Oberti *et al*., 2007). The results are reported in Table 5. As expected, ^{T}Al is ordered at the *T*(1) site, smaller B cations (Mn,Fe,Mg) are ordered at the *M*(4') site and $^{C}R^{3+}$ cations are almost ordered at the *M*(2) site but for a small amount of Al occurring at *M*(3). This was assumed to improve the agreement between the observed and calculated mean bond lengths at the *M*(2) and *M*(3) sites, is in accord with the high Mg content of the sample and may suggest high-*T* crystallization (Oberti *et al*., 1995).

A comparison of the optical and crystallographic properties of the three members related to the hornblende rootname that have been characterized recently is provided in Table 6. In these three hornblende compositions the 2V value drops significantly with increasing Fe content, a feature which might be used for preliminary mineral characterization from petrographic sections. Moreover, changes in the mean bond lengths measured in the strip of octahedra are in accord with changes in the composition of the samples. The $^{C}Al_{1}{}^{C}Fe^{3+}_{1}$ exchange (occurring at the *M*(2) site) and the $^{W}(OH)_{-1}{}^{W}F_{1}$ exchange (occurring at the O(3) site coordinated by two *M*(1) and one *M*(3) cations) describe the transition from magnesio-hornblende to magnesio-ferri-fluoro-hornblende, and lead to an increase in the <*M*(2)–O> distance and a decrease in both <*M*(1)–O> and <*M*(3)–O> distances. In contrast, the $^{C}Mg_{-1}{}^{C}Fe^{2+}_{1}$ exchange (occurring at all the *M*(1,3) sites) and the $^{C}Al_{-1}{}^{C}Fe^{3+}_{1}$ exchange (occurring at the *M*(2) site) describe the transition from magnesio-hornblende to ferro-ferri-hornblende and increases all the <*M*(1,2,3)–O> distances. All these changes are consistent with the differences in ionic radii (Shannon, 1976) of the constituent cations.

The extension of the double chain of tetrahedra along *c*, as measured by the O(5)–O(6)–O(5) angle, is lower in magnesio-hornblende than in ferro-ferri-hornblende; the more extended double chain of tetrahedra promotes linkage with the strip of octahedra where Mg and Al are replaced, respectively, by the larger Fe^{2+} and Fe^{3+} cations. However, the O(5)–O(6)–O(5) angle in magnesio-ferri-fluoro-hornblende (where the ^{T}Al content is 0.37 apfu larger) is very similar to that in ferro-ferri-hornblende (Oberti *et al.*, 2016*b*).

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Supplementary material

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