



Plumbogottlobite, $\text{PbMg}(\text{VO}_4)(\text{OH})$, the Pb analogue of gottlobite and the Mg analogue of descloizite

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Abstract. Plumbogottlobite (IMA 2025-075), $\text{PbMg}(\text{VO}_4)(\text{OH})$, is a new mineral from the Glücksstern mine, Gottlob Hill, Friedrichroda, Gotha District, Thuringia, Germany; it is a late-stage, low-temperature hydrothermal mineral occurring on baryte and hausmannite. Plumbogottlobite forms orange-brown tablets up to about 0.2 mm in diameter. The mineral has a light-orange-brown streak, adamantine lustre, a Mohs hardness of ~ 4 to 4.5, brittle tenacity, irregular to conchoidal fracture, no cleavage, and a calculated density of 5.359 g cm^{-3} . Optically, plumbogottlobite crystals are biaxial (–), with $2V = 84(1)^\circ$. The empirical formula from electron probe microanalyses based on 5 O *apfu* is $(\text{Pb}_{0.89}\square_{0.11})_{\Sigma 1.00}(\text{Mg}_{0.77}\text{Cu}_{0.19}\text{Mn}_{0.09}^{2+})_{\Sigma 1.05}(\text{VO}_4)(\text{OH}) (+0.12 \text{ H for charge balance})$. Plumbogottlobite is orthorhombic with space group *Pnma* and single-crystal unit-cell parameters $a = 7.6104(7)$, $b = 6.1091(6)$, $c = 9.3968(8) \text{ \AA}$, $V = 436.88(7) \text{ \AA}^3$, and $Z = 4$. The crystal structure is refined to $R_1 = 0.0302$ for 429 reflections with $I > 2\sigma_I$. The mineral is the Pb analogue of gottlobite and the Mg analogue of descloizite.

1 Introduction

Dorđević et al. (2016) noted 17 minerals and 12 synthetic compounds with the descloizite–adelite structure topology and provided the general formula $M1^{1+,2+}M2^{2+,3+}(\text{OH},\text{O})[\text{X}^{4+,5+,6+}(\text{O}_4,\text{O}_3\text{OH})]$, where $M1 = \text{Na}^+, \text{Ca}^{2+}, \text{Cd}^{2+}, \text{Hg}^{2+}, \text{Pb}^{2+}$; $M2 = \text{Mg}^{2+}, \text{Al}^{3+}, \text{Mn}^{2+,3+}, \text{Fe}^{2+}, \text{Co}^{2+}, \text{Ni}^{2+}, \text{Cu}^{2+}, \text{Zn}^{2+}$; and $\text{X} = \text{Si}^{4+}, \text{P}^{5+}, \text{V}^{5+}, \text{As}^{5+}, \text{Mo}^{6+}$. Among the minerals are eight arsenates, seven vanadates, and two silicates. One of the vanadates, gottlobite, $\text{CaMg}(\text{VO}_4)(\text{OH})$, has only been found at the Glücksstern mine, Gottlob Hill, Thuringia, Germany. In examining apparent gottlobite crystals from the Glücksstern mine, we found them to be the Pb analogue of the mineral, with the ideal formula $\text{PbMg}(\text{VO}_4)(\text{OH})$.

The new mineral is named plumbogottlobite based on it being the Pb analogue of gottlobite (Witzke et al., 2000). Note that we chose this name rather than magnesiodescloizite because the mineral is virtually identical in appearance to

gottlobite and occurs in the same general mineral assemblage at the Glücksstern mine. The mineral and its name have been approved by the IMA Commission on New Minerals, Nomenclature and Classification (CNMNC), proposal IMA2025-075 (Warr symbol: Pgot). The holotype specimen is deposited in the collections of the Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, CA 90007, USA, catalogue number 77403.

2 Occurrence and associated minerals

Plumbogottlobite was found on the dumps of the Glücksstern mine, Gottlob Hill, Friedrichroda, Gotha District, Thuringia, Germany ($50^\circ 51' 6'' \text{ N}$, $10^\circ 34' 10'' \text{ E}$). The Glücksstern mine was operated for manganese and iron until its closure in 1855 (Scheven, 1990). The mine is also the type locality for crednerite, CuMnO_2 (Rammelsberg, 1849); gottlobite, $\text{CaMg}(\text{VO}_4)(\text{OH})$ (Witzke et al., 2000); vésigniéite, $\text{BaCu}_3(\text{VO}_4)_2(\text{OH})_2$ (Guillemin, 1955); and wakefieldite-

Table 1. Analytical data (wt %) for plumbogottlobite.

Constituent	Mean	Range	SD	Standard	Normalised
PbO	52.47	51.80–53.41	0.69	PbS	56.48
MgO	8.20	8.00–8.38	0.15	Forsterite	8.82
MnO	1.69	1.58–1.88	0.14	Mn ₂ SiO ₄	1.81
CuO	3.94	3.60–4.12	0.24	Cu metal	4.24
V ₂ O ₅	23.96	23.85–24.06	0.09	V ₂ O ₅	25.79
H ₂ O*					2.85
Total					99.99

* Based on the structure (V = 1 and O = 5).

Table 2. Powder X-ray diffraction data (*d* in Å) for plumbogottlobite (*I*_{calc} > 1.5).

<i>I</i> _{obs}	<i>d</i> _{obs}	<i>d</i> _{calc}	<i>I</i> _{calc}	<i>hkl</i>	<i>I</i> _{obs}	<i>d</i> _{obs}	<i>d</i> _{calc}	<i>I</i> _{calc}	<i>hkl</i>
		5.914	3	1 0 1			1.764	13	4 0 2
53	5.115	5.122	57	0 1 1	25	1.755	1.748	11	1 1 5
20	4.675	4.698	27	0 0 2			1.724	3	3 0 4
39	4.244	4.249	37	1 1 1			1.685	3	2 0 5
17	3.959	3.998	16	1 0 2			1.677	11	2 3 2
25	3.508	3.527	22	2 0 1	55	1.660	1.666	15	1 3 3
18	3.370	3.345	15	1 1 2			1.656	32	3 2 3
100	3.230	3.230	100	2 1 0	14	1.612	1.615	15	4 2 0
38	3.060	3.055	36	0 2 0	14	1.564	1.566	19	1 2 5
		2.957	3	2 0 2	14	1.524	1.527	14	0 4 0
46	2.887	2.897	46	1 0 3			1.510	10	3 0 5
33	2.705	2.714	30	1 2 1	12	1.503	1.504	5	3 3 2
43	2.651	2.662	50	2 1 2			1.501	2	3 2 4
46	2.612	2.617	56	1 1 3			1.475	3	2 2 5
10	2.556	2.561	17	0 2 2	8	1.464	1.466	5	3 1 5
7	2.434	2.449	5	3 0 1			1.459	2	5 1 1
		2.427	4	1 2 2			1.453	2	0 4 2
		2.418	2	2 0 3			1.427	3	1 4 2
		2.382	3	2 2 0			1.416	6	3 3 3
42	2.303	2.309	39	2 2 1	23	1.410	1.409	14	2 1 6
		2.273	3	3 1 1			1.402	4	2 4 1
		2.245	12	1 0 4			1.394	2	0 2 6
20	2.233	2.232	7	3 0 2	6	1.385	1.381	2	0 3 5
69	2.102	2.102	42	1 2 3			1.375	5	4 3 1
		1.990	6	0 3 1			1.359	5	1 3 5
9	1.973	1.971	7	3 0 3	10	1.358	1.354	5	3 2 5
		1.925	5	1 3 1			1.351	8	1 4 3
13	1.901	1.903	12	4 0 0	9	1.341	1.336	8	5 1 3
		1.876	16	3 1 3			1.316	2	3 3 4
20	1.869	1.862	5	0 2 4	4	1.311	1.311	2	0 1 7
		1.815	3	1 3 2			1.306	2	4 1 5
		1.809	6	1 2 4			1.296	2	3 4 1
38	1.793	1.802	4	3 2 2					
		1.795	22	2 3 0					
		1.784	11	4 1 1					

relatively low power of 2 mW, whereas the descloizite spectrum was successfully recorded at 16 mW. The descloizite spectrum was chosen for comparison because of the mineral's similar composition, PbZn(VO₄)(OH), and equivalent structure.

The spectrum of plumbogottlobite is very similar to that of descloizite. A broad, weak band is seen in both spec-

tra in the OH stretching region. The very weak feature at about 1550 cm⁻¹ is probably an overtone. Between 1000 and 200 cm⁻¹, both spectra are dominated by bands related to the stretching and bending vibrations of the VO₄ tetrahedron. The mode assignments shown in Fig. 3 are based on Frost et al. (2001), Martens et al. (2003), and Đorđević et al. (2016).

Table 3. Data collection and structure refinement for plumbogottlobite.

Diffractometer	Rigaku R-Axis Rapid II
X-ray radiation	MoK α ($\lambda = 0.71075 \text{ \AA}$)
Temperature	293(2) K
Structural formula	(Pb _{0.941} □ _{0.059})(Mg _{0.700} Cu _{0.300})(VO ₄)(OH) (incl. unlocated H)
Space group	<i>Pnma</i> (no. 62)
Unit-cell dimensions	$a = 7.6104(7) \text{ \AA}$ $b = 6.1091(6) \text{ \AA}$ $c = 9.3986(8) \text{ \AA}$
<i>V</i>	436.88(7) \AA^3
<i>Z</i>	4
Density (for above formula)	5.516 g cm ⁻³
Absorption coefficient	39.753 mm ⁻¹
<i>F</i> (000)	632.7
Crystal size	120 × 80 × 60 μm
θ range	2.17 to 25.03°
Index ranges	$-9 \leq h \leq 9$, $-7 \leq l \leq 7$, $-11 \leq k \leq 11$
Refls collected/unique	7391/430; $R_{\text{int}} = 0.142$
Reflections with $I > 2\sigma_I$	429
Completeness to $\theta = 25.03^\circ$	100 %
Refinement method	Full-matrix least-squares on F^2
Parameters/constraints	49/0
GoF	1.309
Final <i>R</i> indices [$I > 2\sigma_I$]	$R_1 = 0.0302$, $wR_2 = 0.0754$
<i>R</i> indices (all data)	$R_1 = 0.0304$, $wR_2 = 0.0755$

Note that $R_{\text{int}} = \Sigma |F_o^2 - F_c^2(\text{mean})| / \Sigma [F_o^2]$. GoF = $S = \{\Sigma [w(F_o^2 - F_c^2)^2] / (n - p)\}^{1/2}$. $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$. $wR_2 = \{\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]\}^{1/2}$; $w = 1 / [\sigma^2(F_o^2) + (aP)^2 + bP]$, where a is 0, b is 8.134, and P is $[2F_c^2 + \text{Max}(F_o^2, 0)] / 3$.

6 Crystallography

6.1 X-ray powder diffraction

X-ray powder diffraction data were recorded using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer with monochromatised MoK α radiation. A Gandolfi-like motion on the ϕ and ω axes was used to randomise the sample. Observed d values and intensities were derived by profile fitting using JADE Pro software (Materials Data, Inc.). The calculated intensities were calculated from the structure, also using JADE Pro software. Data are given in Table 2. The unit-cell parameters refined from the powder data using JADE Pro with whole-pattern fitting (space group *Pnma*)

are $a = 7.599(12)$, $b = 6.118(10)$, $c = 9.394(15) \text{ \AA}$, and $V = 436.7(10) \text{ \AA}^3$.

6.2 Single-crystal diffraction

Single-crystal X-ray studies were also done using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer with monochromatised MoK α radiation. The Rigaku CrystalClear software package was used for processing the structure data, including the application of a numerical absorption correction. Note that an empirical absorption correction using the multi-scan method resulted in an almost identical R_{int} . The relatively high R_{int} is probably due to the presence of a small satellite crystal. Useful data could only be obtained out to $\theta = 25^\circ$, which accounts for the rela-

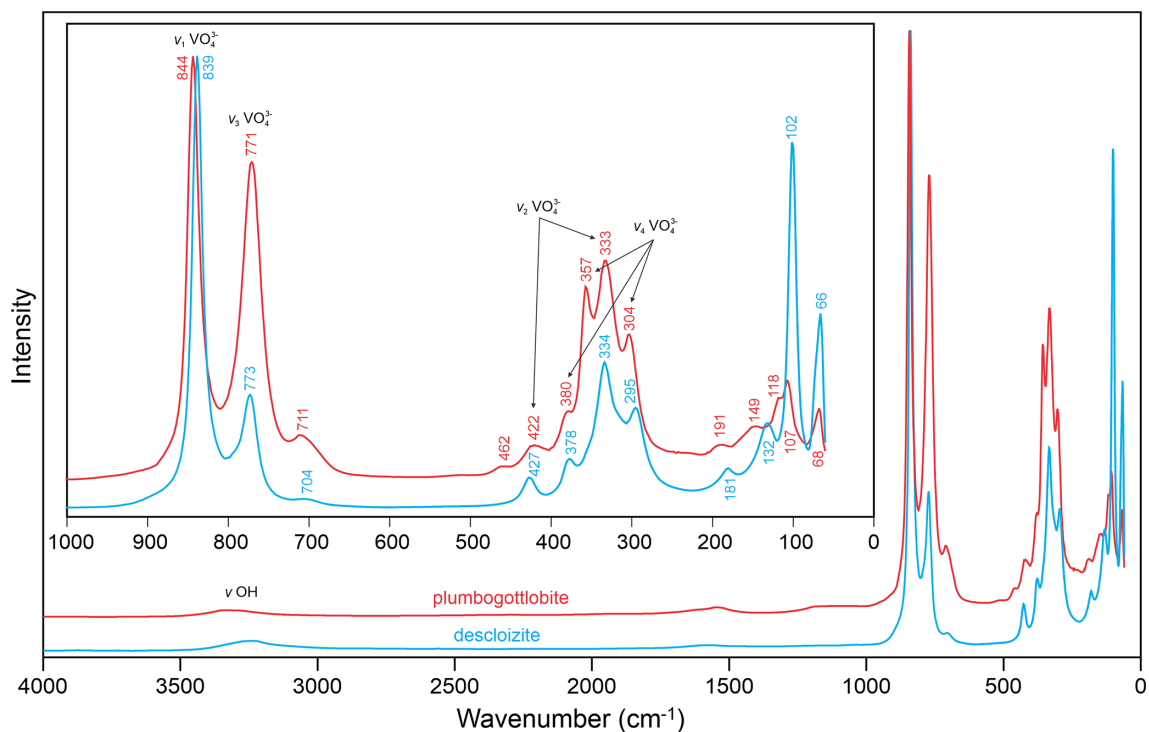


Figure 3. The Raman spectra of plumbogottlobite and descloizite recorded with a 532 nm laser.

Table 4. Refined atom coordinates, displacement parameters (\AA^2), and site occupancies for plumbogottlobite.

	x/a	y/b	z/c	U_{eq}	Occupancy	
Pb	0.12856(7)	0.25	0.17602(6)	0.0178(3)	0.941(12)	
Mg	0.5	0	0	0.0132(11)	$\text{Mg}_{0.700(17)}\text{Cu}_{0.300(17)}$	
V	0.8639(3)	0.75	0.1905(2)	0.0139(10)		
O1	0.8737(8)	0.5114(14)	0.2947(8)	0.0196(18)		
O2	0.0406(13)	0.75	0.0887(11)	0.024(2)		
O3	0.6856(12)	0.75	0.0719(10)	0.016(2)		
OH	0.6501(12)	0.25	0.0724(10)	0.015(2)		
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pb	0.0135(4)	0.0255(5)	0.0145(4)	0	0.00020(19)	0.000
Mg	0.0115(15)	0.0149(17)	0.0132(15)	-0.0005(12)	-0.0013(11)	-0.0013(11)
Cu	0.0115(15)	0.0149(17)	0.0132(15)	-0.0005(12)	-0.0013(11)	-0.0013(11)
V	0.0121(14)	0.0151(16)	0.0147(14)	0	-0.0020(8)	0.000
O1	0.018(4)	0.020(4)	0.021(3)	0.000(3)	-0.003(3)	-0.003(3)
O2	0.016(5)	0.033(6)	0.023(5)	0	0.004(4)	0.000
O3	0.014(5)	0.018(5)	0.015(5)	0	-0.005(4)	0.000
OH	0.015(4)	0.018(5)	0.012(5)	0	0.004(4)	0.000

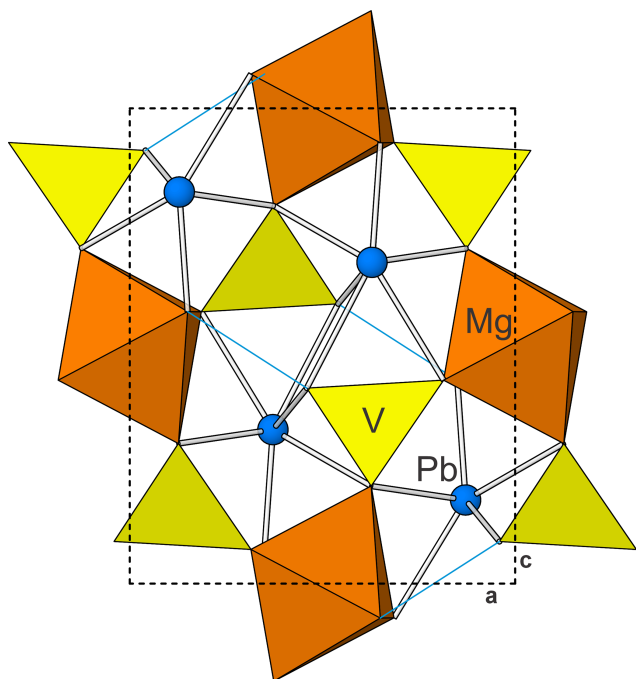
Table 5. Selected bond distances (Å) for plumbogottlobite.

Pb–OH	2.370(9)	Mg–OH($\times 2$)	2.025(6)	V–O2	1.651(10)
Pb–O1($\times 2$)	2.471(7)	Mg–O1($\times 2$)	2.156(7)	V–O3	1.756(9)
Pb–O3	2.725(9)	Mg–O3($\times 2$)	2.187(7)	V–O1($\times 2$)	1.758(8)
Pb–O1($\times 2$)	2.749(7)	<Mg–O>	2.157	<V–O>	1.722
Pb–O2	2.801(10)				
Pb–O2($\times 2$)	3.233(3)	Hydrogen bond			
<Pb–O _{short} >	2.437	OH \cdots O2	1.799(13)		
<Pb–O _{long} >	2.915				

Table 6. Bond valence analysis for plumbogottlobite. Values are expressed in valence units (vu).

	Pb (Pb _{0.941} □ _{0.059})	Mg (Mg _{0.700} Cu _{0.300} ²⁺)	V	H	Σ
O1	0.35 $\times 2$ ↓, 0.19 $\times 2$ ↓	0.28 $\times 2$ ↓	1.11		1.93
O2	0.17, 0.06 $\times 2$ ↓→		1.46	0.18	1.95
O3	0.20	0.26 $\times 2$ ↓→	1.12 $\times 2$ ↓		1.84
OH	0.44	0.39 $\times 2$ ↓→		−0.18	1.02
Σ	2.01	1.86	4.81		

Bond valence parameters are from Gagné and Hawthorne (2015). Hydrogen bond valence is based on the O \cdots O bond lengths from Ferraris and Ivaldi (1988); the negative value indicates donated bond valence.

**Figure 4.** The structure of plumbogottlobite viewed along [010], the chain direction. The hydrogen bond is shown as turquoise lines. The unit-cell outline is shown with dashed lines.

tively low data-to-parameter ratio. The structure was solved in space group *Pnma* using the intrinsic-phasing algorithm of SHELXT (Sheldrick, 2015a). SHELXL-2016 (Sheldrick, 2015b) was used for the refinement of the structure. We also attempted a structure solution and refinement in space group *P2₁2₁2₁*, the space group reported for gottlobite by Đorđević et al. (2016). The refinement provided approximately the same final *R*₁; however, the O4 site in that refinement could not be refined anisotropically without becoming non-positive definite (NPD), and checkcif provided a level-B alert, indicating that the correct space group was probably *Pnma*.

The structure solution in *Pnma* located all non-hydrogen sites, which were successfully refined with anisotropic displacement parameters. The occupancy of the Pb site was refined to 0.941(12). This compares reasonably well with the results of the EPMA, which provided 0.89 Pb *apfu*; however, because the EPMA showed an excess of 0.05 cations assignable to the Mg site, the possibility exists that a small amount of Mn²⁺ could be hosted in the Pb site. The refined site-scattering value of 308.64 *e* for the Pb site is consistent with the site occupancy (Pb_{0.93}Mn_{0.05}□_{0.02}). The Mg site was refined with joint occupancy by Mg and Cu resulting in an occupancy of Mg_{0.700(17)}Cu_{0.300(17)} for a site-scattering value of 68.40 *e*. If 0.05 Mn *apfu* is assigned to the Pb site, the empirical formula based on the EPMA has (Mg_{0.77}Cu_{0.19}Mn_{0.04}²⁺) in the Mg site, which yields a site-scattering value of 63.00 *e*. This suggests that the structure crystal contains less Mg and more Cu and/or Mn than provided by the EPMA. For example, (Mg_{0.68}Cu_{0.24}Mn_{0.08}²⁺) in the Mg site would provide a scattering value of 68.48 *e*. Ef-

Table 7. Selected data for gottlobite, plumbogottlobite, and descloizite.

	Gottlobite	Plumbogottlobite	Descloizite
Formula	CaMg(VO ₄)(OH)	PbMg(VO ₄)(OH)	PbZn(VO ₄)(OH)
Space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>Pnma</i>	<i>Pnma</i>
Unit-cell parameters	<i>a</i> = 7.501(4) Å <i>b</i> = 9.010(7) Å <i>c</i> = 5.941(4) Å <i>V</i> = 401.5(3) Å ³	<i>a</i> = 7.6104(7) Å <i>b</i> = 6.1091(6) Å <i>c</i> = 9.3968(8) Å <i>V</i> = 436.88(6) Å ³	<i>a</i> = 7.593(2) Å <i>b</i> = 6.057(1) Å <i>c</i> = 9.416(2) Å <i>V</i> = 433.1(2) Å ³
<i>Z</i>	4	4	4
Density _{calc}	3.46 g cm ⁻³	5.359 g cm ⁻³	6.202 g cm ⁻³
Reference	Witzke et al. (2000)	This study	Hawthorne and Faggiani (1979)

forts to locate the H site were unsuccessful. The data collection and refinement details are given in Table 3, atom coordinates and displacement parameters are given in Table 4, selected bond distances are given in Table 5, and a bond valence analysis is given in Table 6. The bond valence analysis (using the refined site occupancies) clearly indicates that OH is OH⁻, and all other O sites are O²⁻.

7 Description of the structure

Plumbogottlobite has the same structure as descloizite, PbZn(VO₄)(OH), and other minerals with the descloizite structure type. It is the Pb analogue of gottlobite and the Mg analogue of descloizite; selected data are presented in Table 7. As noted by Đorđević et al. (2016), gottlobite, CaMg(VO₄)(OH), has an adelite-type structure with space group *P*2₁2₁2₁, which is topologically equivalent to the descloizite structure. Đorđević et al. (2016) noted that most phases with the descloizite–adelite structure topology that have the descloizite structure type are lead vanadates.

In the structure of plumbogottlobite, edge-sharing chains of MgO₄(OH)₂ octahedra running parallel to [010] are corner-linked by VO₄ tetrahedra to form a three-dimensional framework. Cavities within the framework host Pb²⁺ cations. The Pb²⁺ is nine-coordinated, with three short bonds (2.37–2.47 Å) on one side and six longer bonds (2.73–3.23 Å) on the other, clearly showing the 6s² lone-pair electrons of Pb²⁺ to be stereoactive. The structure is shown in Fig. 4.

Data availability. Crystallographic data for plumbogottlobite are available in the Supplement.

Supplement. The supplement related to this article is available online at <https://doi.org/10.5194/ejm-38-209-2026-supplement>.

Author contributions. ARK oversaw the research, determined the physical and optical properties, did the Raman spectroscopy, did the X-ray diffraction studies, and wrote the paper. JD conducted initial characterisation studies on the mineral and identified it as a potential new species. CM did the electron probe microanalyses.

Competing interests. The contact author has declared that none of the authors has any competing interests.

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