TELLUROMANDARINOITE, A NEW TELLURITE MINERAL FROM THE EL INDIO-TAMBO MINING PROPERTY, ANDES MOUNTAINS, CHILE

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Abstract

Telluromandarinoite, a tellurite, is a new mineral species from the Wendy open pit, Tambo mine, El Indio-Tambo mining property, Coquimbo Province, Chile. The ideal endmember telluromandarinoite formula is $Fe^{3+}_2Te^{4+}_3O_9 \cdot 6H_2O$ and it is the Te^{4+} analogue of the selenite mineral mandarinoite, $Fe^{3+}_2Se^{4+}_3O_9 \cdot 6H_2O$. These deposits are located in rhyolitic and dacitic pyroclastic volcanic rocks of Tertiary age (8–11 Ma) that are strongly hydrothermally altered. The mineralization in the Tambo area is characterized by high-level epithermal veins and breccias located along roughly east–west structures. Hydrothermal breccias consisting of silicified clasts of dacite tuffs cemented by a silica/barite/alunite matrix are common at the occurrence. In fact, all studied specimens containing tellurite mineralization are associated with alunite. Telluromandarinoite is translucent, pale green, with a white streak and vitreous luster. It forms as individual platy crystals, 0.2 mm or less in size, but more commonly as aggregates of platy crystals. The crystals are too small to allow a Mohs hardness determination; they are brittle with an uneven fracture and no observed cleavage or parting. Telluromandarinoite is biaxial positive with $\alpha = 1.750(3)$, $\beta = 1.807(3)$, and $\gamma = 1.910(5)$, with a calculated $2V = 76.9°$. The optical orientation is $Y = \mathbf{b}$, $\mathbf{c} \wedge Z = 10°$ in obtuse β. No dispersion was noted and no pleochroism was observed. An average of 10 electron microprobe analyses gave SeO_2 22.91, TeO_2 44.30, Fe_2O_3 26.43, and H_2O (calc.) 17.59, total 111.23 wt.%. The mineral loses H_2O in vacuum, so the high totals obtained were expected. The empirical formula (based on 15 O atoms) is $Fe^{3+}_{2.03}(Te^{4+}_{1.71}Se^{4+}_{1.27})_{\Sigma 2.98}O_9 \cdot 6H_2O$ with $Z = 4$, and $D_{calc} = 3.372$ g/cm^3. Spot analyses gave stoichiometries that range from telluromandarinoite $Fe^{3+}_{2.03}(Te^{4+}_{2.12}Se^{4+}_{0.86})_{\Sigma 2.98}O_9 \cdot 6H_2O$ to mandarinoite $Fe^{3+}_{2.07}(Se^{4+}_{1.64}Te^{4+}_{1.31})_{\Sigma 2.95}O_9 \cdot 6H_2O$. A crystal-structure analysis shows the mineral to be monoclinic, space group $P2_1/c$, with a 16.9356(5), b 7.8955(3), c 10.1675(3) Å, β 98.0064(4)°, and V 1346.32(13) Å^3. The strongest lines in the X-ray powder pattern [d in Å,(I),(hkl)] are: 8.431(44)(200), 7.153(100)($\bar{1}$10), 3.5753(41)($\bar{2}$20), 3.4631(21)($\bar{4}$02), 2.9964(34)($\bar{2}$22), 2.8261(19)(412). The crystal structure of telluromandarinoite is similar to that of emmonsite, $Fe^{3+}_2Te^{4+}_3O_9 \cdot 2H_2O$.

Keywords: telluromandarinoite, new mineral species, tellurite, crystal structure, El Indio-Tambo mining property, Chile.

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Introduction

Telluromandarinoite, a new tellurite mineral, occurs in the Wendy open pit, Tambo mine, at the El Indio-Tambo mining property, Coquimbo Province, located in the Chilean Andes, approximately 640 km north of Santiago and 160 km east of La Serena, Chile. Mining claims in the area date from 1967, although full-scale mining did not begin until 1981. The current majority owner of the property is Barrick Gold Corporation of Toronto, which acquired it in late 1994 (P.C. Walford, *pers. commun.*). The holotype specimen was collected in 1992 by Mr. Phillip Walford who was then Vice-President and Chief Geologist for LAC Minerals Ltd., when they owned the mining rights at the mine. He collected most of the study material available from this locality, and discovered the new mineral here named telluromandarinoite, in reference to its tellurium dominant relationship to mandarinoite, a selenite mineral. Mandarinoite was named for the late Dr. Joseph A. Mandarino (Dunn *et al.* 1978). Three other new species were brought to the attention of the senior author. One of the three minerals was described and named walfordite (Back *et al.* 1999); the other two minerals are Fe-tellurites, which have now been described and submitted to the CNMNC for approval.

The new mineral and the mineral name have been approved by the Commission on New Minerals, Names and Classification, IMA (2011-013). Holotype material is housed in the collection of the Royal Ontario Museum, Natural History Department, Mineralogy, under catalogue number M56017. In this paper, we provide the physical and chemical data that establish telluromandarinoite as a new species, and describe its structure and its relationship to the species mandarinoite.

Occurrence

The El Indio-Tambo mining property covers 1295 square kilometers of the El Indio Belt, a prolific gold, silver, and copper district located in Coquimbo Province, Chile, close to the Argentina border in the Andes Mountains (approximately 70° W longitude and 30° S latitude). The property consisted of two mines, the El Indio mine, a porphyry copper-gold deposit, and the Tambo mine, located within five kilometers of each other in the south-central portion of the property, and is at an elevation of approximately 3950 m. The mineralization in the Tambo area is characterized by high-level epithermal veins and breccias located along roughly east–west structures. The Wendy open pit is one of three pits that were worked at the Tambo mine.
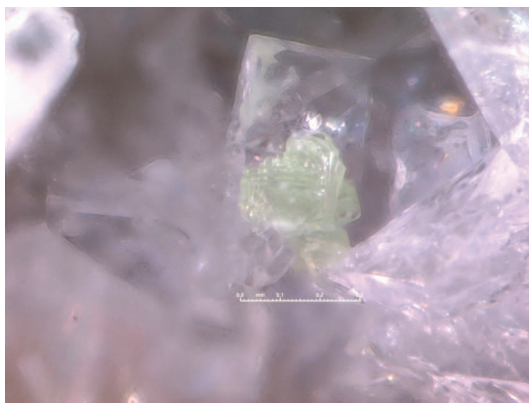

Fig. 1. A cluster of telluromandarinoite crystals with associated alunite matrix (scale bar 0.3 mm).

All mining operations have now closed and the site has been reclaimed.

The regional and local geology of the area was described by Siddeley & Araneda (1986). These deposits are located in rhyolitic and dacitic pyroclastic volcanic rocks of Tertiary age (8–11 Ma) that are strongly hydrothermally altered. The Wendy pit is located on the south flank of Cerro Elefante, which is a north–south elongate accumulation of dacite tuffs. Hydrothermal breccias are a common feature of the Tambo mine, and consist of silicified clasts of dacitic tuffs cemented by silica, barite, and alunite (Siddeley & Araneda 1986).

Telluromandarinoite must be considered to be extremely rare. To date, only a few specimens have been found, each containing only a few milligrams of material. Telluromandarinoite and many other tellurite minerals are found in the interstices of the silicified hydrothermal breccias. Associated minerals are alunite, emmonsite, mackayite, poughite, rodalquilarite, and two Fe-tellurite minerals that have now been submitted to the CNMNC for approval. Other minerals identified from the same environment include barite, gold, jarosite, paratellurite, pyrite, scorodite, tellurite, and walfordite.

Physical and Optical Properties

Telluromandarinoite occurs as isolated platy crystals and also as aggregates of platy crystals. Individual crystals are 0.2 mm or less in size. The crystals are translucent, pale green (Fig. 1), with a white streak and a vitreous luster. Telluromandarinoite exhibits no fluorescence in short- or long-wavelength ultraviolet light. The crystals are too small to allow for the measurement of Mohs hardness; they are brittle with no observed cleavage or parting. The fracture is

irregular, and due to a paucity of material and small grain size, the density could not be measured. The calculated density is 3.372 g/cm^3.

Telluromandarinoite is optically biaxial positive, with $\alpha = 1.750(3)$ and $\beta = 1.807(3)$ measured (589 nm) from a single crystal mounted on a spindle stage, and $\gamma = 1.910(5)$ calculated from retardation measurements using a tilting Berek compensator. Calculated $2V = 76.9°$. The optical orientation is Y = **b**, **c** ˆ Z = 10° in obtuse β. No dispersion was noted and no pleochroism was observed.

CHEMICAL COMPOSITION

Chemical analyses (10) were carried out using a Cameca SX100 electron microprobe (WDS mode, 15 kV, 10 nA, 15 μm beam diameter). The mineral loses H_2O in the vacuum, so the high totals obtained were expected. The sample decrepitated and cracked under the beam (see below). The standards used were synthetic Bi_2Se_3 (Se$L\alpha$), synthetic PbTe (Te$L\alpha$), and fayalite (Fe$K\alpha$).

The stoichiometry for the cations is good. The large range in compositions of the studied material indicates a solid solution ranging from mandarinoite to telluromandarinoite. Vanadium, Cr, Ni, Cu, and Al were below detection limits. H_2O was not determined directly due to the paucity of available material. The presence of H_2O was confirmed on the basis of results of the crystal-structure analysis, with calculated amounts being derived from the refined crystal structure, and by analogy with the Se analogue, mandarinoite. The average result of 10 analyses gave SeO_2 22.91 (14.72–30.25) (sd 6.25), TeO_2 44.30 (34.80–52.86) (7.45), Fe_2O_3 26.43 (25.19–27.54) (0.82), and H_2O (calculated from stoichiometry based on the structure and by analogy with mandarinoite) 17.59, total 111.23 wt.%. Normalized, this gives SeO_2 20.60, TeO_2 39.83, Fe_2O_3 23.76, and H_2O 15.81, total 100.00 wt.%.

The empirical formula (based on 15 O atoms) is $Fe^{3+}_{2.03}(Te_{1.71}Se_{1.27})_{\Sigma2.98}O_9 \cdot 6H_2O$. Spot analyses gave stoichiometries that range from $Fe^{3+}_{2.03}(Te_{2.12}Se_{0.86})_{\Sigma2.98}O_9 \cdot 6H_2O$ to $Fe^{3+}_{2.07}(Se_{1.64}Te_{1.31})_{\Sigma2.95}O_9 \cdot 6H_2O$. The ideal endmember formula is $Fe^{3+}_2Te_3O_9 \cdot 6H_2O$, which requires TeO_2 64.13, Fe_2O_3 21.39, H_2O 14.48, total 100 wt.%.

Gladstone-Dale calculations using the constants of Mandarino (1981) indicate a compatibility of physical and chemical data of 0.020 (excellent).

X-RAY CRYSTALLOGRAPHY AND CRYSTAL-STRUCTURE DETERMINATION

X-ray precession photographs as well as a structure determination showed telluromandarinoite to be mono-

TABLE 1. POWDER X-RAY DATA FOR TELLUROMANDARINOITE AND MANDARINOITE, FOR COMPARISON

telluromandarinoite					mandarinoite	
I_{rel}	I_{calc}	d_{meas}/Å	d^*_{calc}/Å	hkl	I_{rel}	d_{meas}/Å
44	**84**	**8.431**	**8.394**	200	40	8.25
100	100	**7.153**	**7.149**	$\bar{1}$10	100	7.10
10	12	6.248	6.215	011	5	6.14
11	33	5.034	5.032	002	5	4.94
5	7	4.812	4.806	211	5	4.74
5	8	4.345	4.344	$\bar{3}$11	10	4.53
10	24	4.197	4.197	400	10	4.16
					5	3.95
41	**44**	**3.5753**	**3.5746**	$\bar{2}$20	5	3.65
			3.5556	121	50	3.55
21	**49**	**3.4631**	**3.4632**	$\bar{4}$02	40	3.43
7	5	3.3417	3.35	411	5	3.31
10	14	3.0959	3.0901	510	5	3.04
			3.0881	013		
34	**36**	**2.9964**	**2.9974**	$\bar{2}$22	70	2.977
19	**18**	**2.8261**	**2.8266**	412	20	2.804
				502	5	2.741
11	16	2.6239	2.6247	322	10	2.591
					10	2.451
10	9	2.2938	2.2948	$\bar{7}$10		
		2.2920		$\bar{4}$23		
		2.2917		132		
7	6	2.2765	2.2821	$\bar{6}$21	10	2.275
					5	2.195
					5	2.140
8	7	2.0709	2.0717	033		
7	6	2.0517	2.0518	$\bar{2}$33	10	2.042
		2.0501		720		
7	13	1.9676	1.9676	$\bar{1}$15	10	1.964

Note: 114.6 mm Gandolfi camera, Cu$K\alpha$ (Ni filtered) radiation. Film was scanned using an optical scanner calibrated for intensity and peak position using an external silicon standard.
* Calculated from refined cell parameters, $a = 16.945(6)$, $b = 7.902(3)$, $c = 10.159(2)$ Å, and $\beta = 97.82(2)°$.

clinic, with space group $P2_1/c$. The cell parameters from the structure determination are a 16.9356(5), b 7.8955(3), c 10.1675(3) Å, β 98.0064(4)°, and $V = 1346.32(13)$ Å^3, refined using 9288 indexed reflections. X-ray powder-diffraction data collected with a Gandolfi camera, 114.6 mm in diameter, with Cu$K\alpha$ (Ni filtered) radiation are given in Table 1. The film was scanned using an optical scanner calibrated for intensity and peak positions using an external silicon standard. The X-ray data were refined using the PC-based version of the least-squares refinement program of Appleman & Evans (1973). The cell parameters refined from the

TABLE 2. TELLUROMANDARINOITE: DATA COLLECTION AND STRUCTURE
REFINEMENT INFORMATION

Space Group	$P2_1/c$	Measured reflections	15845
a (Å)	16.9356(5)	Unique reflections	3969
b (Å)	7.8955(3)	Observed reflections [$> 4\sigma(F)$]	3283
c (Å)	10.1675(3)	R(int)	0.0161
β (°)	98.0064(4)	Goodness of fit on F^2	1.48
V (Å^3)	1346.32(13)	R index for all data	0.034
μ (mm^{-1})	9.47	R index for observed data	0.032

Ideal unit-cell contents: 4[Fe$^{3+}{}_2$(Te$^{4+}{}_2$Se^{4+}O$_9$)·6H$_2$O]

powder-diffraction data are a 16.9450(6), b 7.9015(3), c 10.1591(2) Å, β 97.49(2)°, and $V = 1347.6(6)$ Å^3.

The single crystal of telluromandarinoite was a fragment measuring $15 \times 40 \times 60$ µm. Intensity data were collected with a fully automated Bruker $P4$ four-circle diffractometer operated at 50 kV and 40 mA, with graphite-monochromated MoKα radiation and a 4K APEX CCD detector mounted at a 5 cm distance from the crystal. A complete sphere of integrated intensities was collected out to $2\theta = 60°$, using 5 s frame counts and a frame width of 0.2°. Data pertinent to the intensity-data collection are given in Table 2. The unit-cell parameters for the single crystal were refined using 9288 indexed reflections.

Reduction of the intensity data, structure determination, and structure refinement were performed with the SHELXTL (Sheldrick 1990) package of computer programs. Data reduction included corrections for background, scaling, and Lorentz-polarization factors. An empirical absorption correction (SADABS, Sheldrick 1998) was applied.

The atomic coordinates for the initial structure solution were those determined by Hawthorne (1984) for the mandarinoite crystal structure. In the final least-squares refinement, all atom positions, except H atoms, were refined with anisotropic displacement-factors. The H atoms were refined with two restrictions: (1) H–O distances of 0.98 Å and (2) isotropic displacement parameters of 0.05 Å^2. Refinement of site occupancy factors (*sof*) indicates that two of the three Te sites are dominated by Te and the third by Se. The refinement indicates a Te-dominant crystal with 1.56 atoms of Te and 1.44 atoms of Se. The weighting scheme is inversely proportional to $\sigma^2(F)$. The addition of a correction for extinction did not improve the refinement. In the last stage of refinement, the electron residuals were +1.19 and –1.53 e$^-$/Å^3. The final positional coordinates and displacement-parameters are given in Table 3 and selected bond lengths and angles in Table 4. Bond valence calculations for telluromandarinoite are presented in Table 5. The
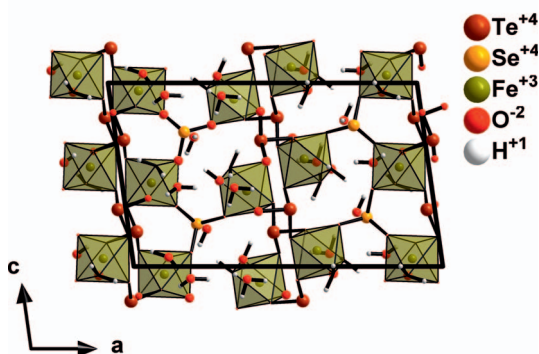

FIG. 2. The framework structure of telluromandarinoite projected along the **b** axis.
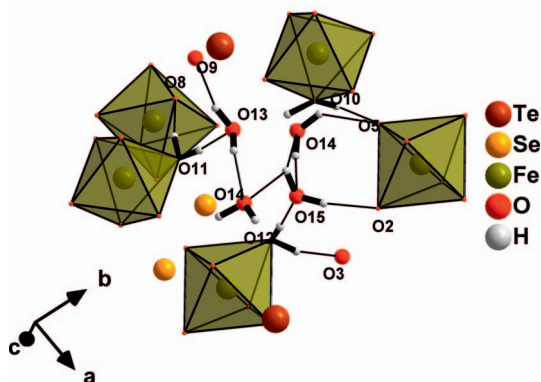

FIG. 3. Hydrogen-bonding scheme in telluromandarinoite.

TABLE 3. TELLUROMANDARINOITE: ATOM COORDINATES AND DISPLACEMENT PARAMETERS

Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{iso}
Te1	0.97522(2)	0.02569(5)	0.31058(3)	0.0159(2)	0.0200(2)	0.0126(2)	0.0042(1)	0.0029(1)	0.0036(1)	0.0161(1)
Se2	0.22425(2)	0.71847(5)	0.73157(4)	0.0129(2)	0.0262(2)	0.0120(2)	0.0023(1)	0.0001(1)	-0.0026(1)	0.0172(1)
Te3	0.53128(2)	0.49290(5)	0.81269(3)	0.0163(2)	0.0181(2)	0.0125(2)	-0.0002(1)	0.0016(1)	0.0044(1)	0.0157(1)
Fe1	0.39975(4)	0.74890(9)	0.91276(6)	0.0124(3)	0.0162(3)	0.0122(3)	0.0011(2)	0.0028(2)	0.0015(2)	0.0135(2)
Fe2	0.90479(4)	0.23678(8)	0.04306(6)	0.0123(3)	0.0158(3)	0.0112(3)	0.0008(2)	0.0020(2)	0.0004(2)	0.0130(2)
O1	0.9771(2)	0.2155(5)	0.4123(4)	0.020(2)	0.025(2)	0.022(2)	-0.007(1)	0.009(1)	-0.005(1)	0.0216(7)
O2	0.0773(2)	-0.0369(5)	0.3716(4)	0.016(2)	0.021(2)	0.022(2)	0.005(1)	-0.003(1)	-0.002(1)	0.0201(7)
O3	0.9971(2)	0.1318(5)	0.1618(3)	0.016(2)	0.026(2)	0.016(2)	0.004(1)	0.004(1)	0.004(1)	0.0190(7)
O4	0.3158(2)	-0.1686(5)	0.7709(3)	0.020(2)	0.019(2)	0.016(2)	0.004(1)	0.001(1)	-0.001(1)	0.0186(7)
O5	0.1926(2)	-0.1738(4)	0.5780(3)	0.0154(2)	0.021(2)	0.016(1)	0.006(1)	0.002(1)	-0.002(1)	0.0175(7)
O6	0.1659(2)	-0.1571(5)	0.8281(4)	0.021(2)	0.0301(2)	0.017(2)	0.003(1)	0.008(1)	0.002(1)	0.0220(7)
O7	0.5199(2)	0.3869(5)	0.6555(4)	0.020(2)	0.026(2)	0.019(2)	-0.004(1)	0.002(1)	0.006(1)	0.0216(7)
O8	0.4282(2)	0.5553(4)	0.8010(3)	0.017(2)	0.019(2)	0.016(1)	-0.002(1)	0.004(1)	0.004(1)	0.0172(6)
O9	0.4766(2)	0.6821(4)	0.0735(3)	0.016(2)	0.020(2)	0.018(2)	0.003(1)	0.002(1)	0.002(1)	0.0180(7)
O10	0.3163(2)	-0.4233(5)	0.9682(4)	0.018(2)	0.020(2)	0.023(2)	0.002(1)	0.010(1)	-0.009(1)	0.0197(7)
O11	0.3570(2)	-0.0756(5)	0.0380(3)	0.022(2)	0.020(2)	0.015(2)	-0.003(1)	-0.001(1)	0.002(1)	0.0197(7)
O12	0.8831(2)	0.0012(5)	-0.0504(4)	0.020(2)	0.018(2)	0.023(2)	-0.002(1)	0.007(1)	0.000(1)	0.0200(7)
O13	0.6390(2)	0.7589(6)	0.0707(4)	0.027(2)	0.028(2)	0.038(2)	0.002(2)	0.008(2)	-0.000(2)	0.0305(9)
O14	0.2537(4)	0.3122(6)	0.2054(5)	0.070(4)	0.031(2)	0.03(3)8	0.004(2)	0.003(2)	0.002(2)	0.047(1)
O15	0.1778(3)	0.2334(6)	0.4333(5)	0.027(2)	0.032(2)	0.047(3)	-0.012(2)	0.007(2)	-0.006(2)	0.036(1)

Site	x	y	z	U_{iso}
H10A	0.275(3)	-0.39(1)	1.023(7)	0.05
H10B	0.324(5)	-0.544(2)	0.95(8)	0.05
H11A	0.387(4)	-0.08(1)	0.127(3)	0.05
H11B	0.355(5)	0.036(4)	-0.004(7)	0.05
H12A	0.934(2)	-0.03(1)	-0.079(7)	0.05
H12B	0.864(4)	-0.089(7)	0.003(7)	0.05

Site	x	y	z	U_{iso}
H13A	0.582(1)	0.75(1)	0.076(8)	0.05
H13B	0.662(4)	0.76(1)	0.164(2)	0.05
H14A	0.224(4)	0.28(1)	0.119(4)	0.05
H14B	0.258(5)	0.435(1)	0.205(8)	0.05
H15A	0.142(4)	0.144(7)	0.394(7)	0.05
H15B	0.191(5)	0.27(1)	0.348(4)	0.05

Note: Site occupancy factors: Te1/Se1 0.614(3)/0.386; Te2/Se2 0.431(2)/0.569; Te3/Se3 0.520(2)/0.48

TABLE 4. TELLUROMANDARINOITE: SELECTED BOND LENGTHS (Å)
AND ANGLES (°)

Te1–O3	1.812(3)	Se2–O6	1.782(4)	Te3–O7	1.791(4)
Te1–O1	1.819(4)	Se2–O4	1.784(4)	Te3–O8	1.802(3)
Te1–O2	1.822(4)	Se2–O5	1.794(3)	Te3–O9	1.819(4)
<Te1–O>	1.8177	<Se2–O>	1.7867	<Te3–O>	1.8040
O1–Te1–O3	96.0(2)	O4–Se2–O6	97.6(2)	O8–Te3–O7	95.0(2)
O2–Te1–O3	96.6(2)	O5–Se2–O6	95.6(2)	O9–Te3–O7	101.8(2)
O2–Te1–O1	95.1(2)	O5–Se2–O4	96.0(2)	O9–Te3–O8	95.4(2)
<O–Te1–O>	95.90	<O–Se2–O>	96.40	<O–Te3–O>	97.40
Fe1–O7	1.945(4)	Fe2–O1	1.965(3)		
Fe1–O4	1.989(4)	Fe2–O2	1.991(4)		
Fe1–O8	2.003(3)	Fe2–O6	1.995(4)		
Fe1–O9	2.012(4)	Fe2–O3	2.016(4)		
Fe1–O11	2.079(4)	Fe2–O5	2.041(3)		
Fe1–O10	2.095(4)	Fe2–O12	2.097(4)		
<Fe1–O>	2.1553	<Fe2–O>	2.0175		
O4–Fe1–O7	91.3(2)	O2–Fe2–O1	93.0(2)		
O8–Fe1–O7	89.4(2)	O6–Fe2–O1	88.8(1)		
O9–Fe1–O7	91.8(2)	O3–Fe2–O1	93.0(1)		
O11–Fe1–O7	99.5(2)	O5–Fe2–O1	87.1(2)		
O8–Fe1–O4	92.5(2)	O6–Fe2–O2	93.8(2)		
O11–Fe1–O4	87.2(1)	O3–Fe2–O2	92.9(2)		
O10–Fe1–O4	88.1(2)	O5–Fe2–O2	90.8(1)		
O9–Fe1–O8	94.7(1)	O3–Fe2–O6	87.9(1)		
O10–Fe1–O8	83.2(2)	O5–Fe2–O6	89.8(2)		
O11–Fe1–O9	85.3(1)	O12–Fe2–O6	86.2(2)		
O10–Fe1–O9	89.7(2)	O12–Fe2–O3	88.8(2)		
O10–Fe1–O11	87.8(2)	O12–Fe2–O5	87.6(1)		
<O–Fe–O>	90.04	<O–Fe2–O>	89.98		

D–H	d(D–H)	d(H⋯A)	<DHA	d(D⋯A)	A
O10–H10A	0.98	1.66	165	2.62	O5
O10–H10B	0.98	1.84	167	2.80	O13
O11–H11A	0.98	1.81	168	2.78	O8
O11–H11B	0.98	1.76	174	2.74	O13
O12–H12A	0.98	1.72	162	2.67	O3
O12–H12B	0.98	1.74	168	2.70	O15
O13–H13A	0.98	1.86	165	2.82	O9
O13–H13B	0.98	1.84	152	2.74	O14
O14–H14A	0.98	1.94	167	2.91	O15
O14–H14B	0.98	2.14	153	3.04	O4
O14–H14B	0.98	2.46	137	3.25	O5
O15–H15A	0.98	1.80	163	2.75	O2
O15–H15B	0.98	1.94	159	2.87	O14

calculations for the Te and Se positions are weighted using the *sof* data obtained from the structure determination. These calculations indicate a good fit with the data. Tables listing the observed and calculated structure factors and a .cif file may be obtained from the Depository of Unpublished Data, on the MAC web site [document: telluromandarinoite CM55-1_10.3749/canmin.1500014].

DESCRIPTION OF THE STRUCTURE

Telluromandarinoite is isostructural with mandarinoite (Hawthorne 1984). The telluromandarinoite crystal structure (Fig. 2) has two Fe^{3+} atomic sites; Fe1 is coordinated by four O atoms and two water groups and Fe2 is coordinated by five O atoms and one water group; both polyhedra are insular pseudo-

TABLE 5. BOND-VALENCE CALCULATIONS USING THE *sof* FROM THE STRUCTURE DETERMINATION FOR THE Te AND Se POSITIONS

	O1	O2	O3	O4	O5	O6	O7	O8	O9	O10	O11	O12	Σ
Te1/Se1	1.32	1.30	1.34	-	-	-	-	-	-	-	-	-	3.96
Se2/Te2	-	-	-	1.33	1.31	1.34	-	-	-	-	-	-	3.98
Te3/Se3	-	-	-	-	-	-	1.37	1.33	1.27	-	-	-	3.97
Fe1	-	-	-	0.54	-	-	0.60	0.52	0.50	0.40	0.42	-	2.98
Fe2	0.57	0.54	0.50	-	0.47	0.53	-	-	-	-	-	0.40	3.01
Σ	1.89	1.84	1.84	1.87	1.78	1.87	1.97	1.85	1.77	0.40	0.42	0.40	

The bond-valence calculations were done using the equation and constants of Brese & O'Keeffe (1991); $V_{ij} = \exp [(R_{ij} - d_{ij})/b]$, where $b = 0.37$ Å. Bond valences are expressed in valence units (*vu*).

octahedral polyhedra. In addition there are two $(Te,Se)^{4+}$ atom sites and one $(Se,Te)^{4+}$ atom site. Typical of a tellurite anion, they form a trigonal pyramid with Te at the apex. On the side opposite the trigonal base there is an 'invisible' non-bonding pair of electrons that manifests itself as an apparent 'hole' in the structure. The insular $[FeΦ_6]$ octahedra ($Φ = O$ atom or water group) and insular $[TeO_3]$ trigonal pyramids cross-link corners, forming a framework structure. In addition to the three water groups bonded to Fe atoms, there are three other water groups that are not bonded to any cation. Their atom positions are well-defined in the framework channels that parallel the **c** axis. The three water groups are held in place *via* a complex H-bonding scheme that is shown in Figure 3. These water groups are stable under exposure to the X-ray beam, but they are lost under vacuum conditions in the electron microprobe.

Although the telluromandarinoite structure is unique, there are some comparable features in the emmonsite structure (Pertlik 1978). Emmonsite, $Fe^{3+}_2Te^{4+}_3O_9 \cdot 2H_2O$, has the same proportions of cations as telluromandarinoite, $Fe^{3+}_2Te^{4+}_3O_9 \cdot 6H_2O$, but fewer water groups. Both structures are frameworks of cross-linked $[FeO_6]$ octahedra and $[TeO_3]$ trigonal pyramids. In both structures the $[FeO_6]$ octahedra are in parallel rows, along the **c** axis in telluromandarinoite and along [011] in emmonsite. In telluromandarinoite pairs of parallel rows of $[FeO_6]$ octahedra are offset by one-half the *c* parameter while in emmonsite the parallel rows are stacked on top of each other. The water groups were not determined in the emmonsite structure, but one could presume they would reside in the channels along the **a** axis, (Fig. 4), similar to the three water groups that lie in the **c**-axis channels of telluromandarinoite. The most fundamental difference in the two structures is the disposition of the $[FeO_6]$ octahedra; in telluromandarinoite they are insular and in emmonsite they are dimers.
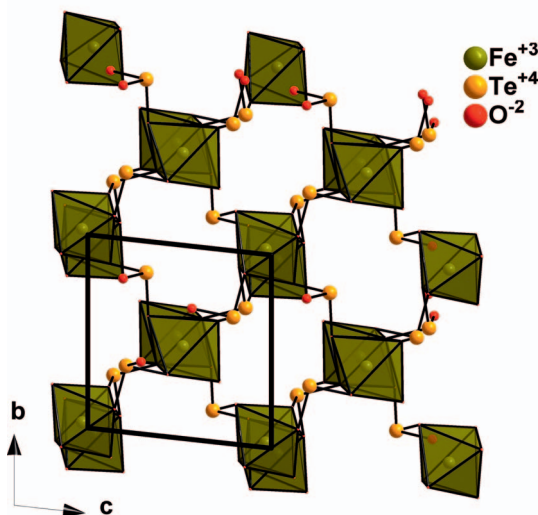

EMMONSITE

Fe⁺³
Te⁺⁴
O⁻²

FIG. 4. The framework structure of emmonsite projected along the **a** axis.

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