American Mineralogist, Volume 97, pages 1627–1634, 2012

Crystal chemistry of Bi- and Mn-bearing vesuvianite from Långban, Sweden

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Abstract

Red vesuvianite crystals occur with hausmanite and calcite in a hand specimen from Långban, Sweden. Backscattered electron imaging revealed that a very few of the vesuvianite crystals exhibit cores of higher average atomic number (vesuvianite I) than the bulk (vesuvianite II). Average electron microprobe compositions of vesuvianite I show 3.32 wt% MnO (1.43 Mn^{2+} apfu), 3.13 wt% Bi_2O_3 (0.41 Bi^{3+} apfu), 0.82 wt% Cl (0.71 Cl apfu), and 0.56 wt% As_2O_5 (0.15 As^{5+} apfu). The average vesuvianite II composition shows considerably more Mn (4.14 wt% MnO, or 1.76 Mn^{2+} apfu) but less Bi (0.62 wt% Bi_2O_3, or 0.08 Bi^{3+} apfu) and Cl (0.13 wt% Cl, or 0.11 Cl apfu) and about the same amount of As (0.62 wt% As_2O_5, or 0.16 As^{5+} apfu). The crystal structures of vesuvianite I (a = 15.595, c = 11.779 Å) and II (a = 15.585, c = 11.778 Å) were refined in space group $P4/nnc$ to R_1 values of 0.0445 and 0.0167, respectively. The results show Bi at the new Bi3 position and Cl at the new Cl site; Bi3 can only be occupied when there is a vacancy at the nearby (~0.4 Å) X3 position, and Cl when there is a vacancy at the nearby (~0.4–0.5 Å) O10 position. Bond distances and site occupancies suggest that the Cl atom at the Cl site is bonded to the Bi atom at the Bi3 position when it is occupied. Arsenic occupies the T1 site and is coordinated by oxygen atoms at two O7B and two O11 positions. Manganese replaces Ca at the X1 and X2 position and dominates the Y1 position in vesuvianite I, whereas in vesuvianite II it replaces Ca at the X1 site and fills the Y1A position. In both structures Mn also occurs subordinate to Al + Mg at the Y3 position. Bond-valence analysis indicates that the Mn at the Y1 and Y1A positions is divalent rather than trivalent as required for manganvesuvianite.

Keywords: Vesuvianite, Långban, manganese, bismuth, arsenic, crystal structure

Introduction

Vesuvianite is a rock-forming or accessory silicate mineral found in metamorphic rocks, rodingites, and altered alkaline rocks. From a crystal-chemical point of view the formula of vesuvianite may be written as $X_{19}Y_{13}Z_{18}O_{69}(OH,F)_9$, where X are seven- to ninefold-coordinated, Y has octahedral or square pyramidal coordination, and Z represents tetrahedral coordination. The X positions are commonly occupied by Ca; the Y sites by Al, Mg, and Fe; and the Z positions by Si. The vesuvianite structure (Fig. 1) is closely related to that of grossular, but differs from it by having additional X4 and Y1 sites (site nomenclature that of Groat et al. 1992a), the latter with square pyramidal coordination, at various levels on the fourfold axes. It is assumed that the X4 and Y1 periodicity is preserved within a single channel, but

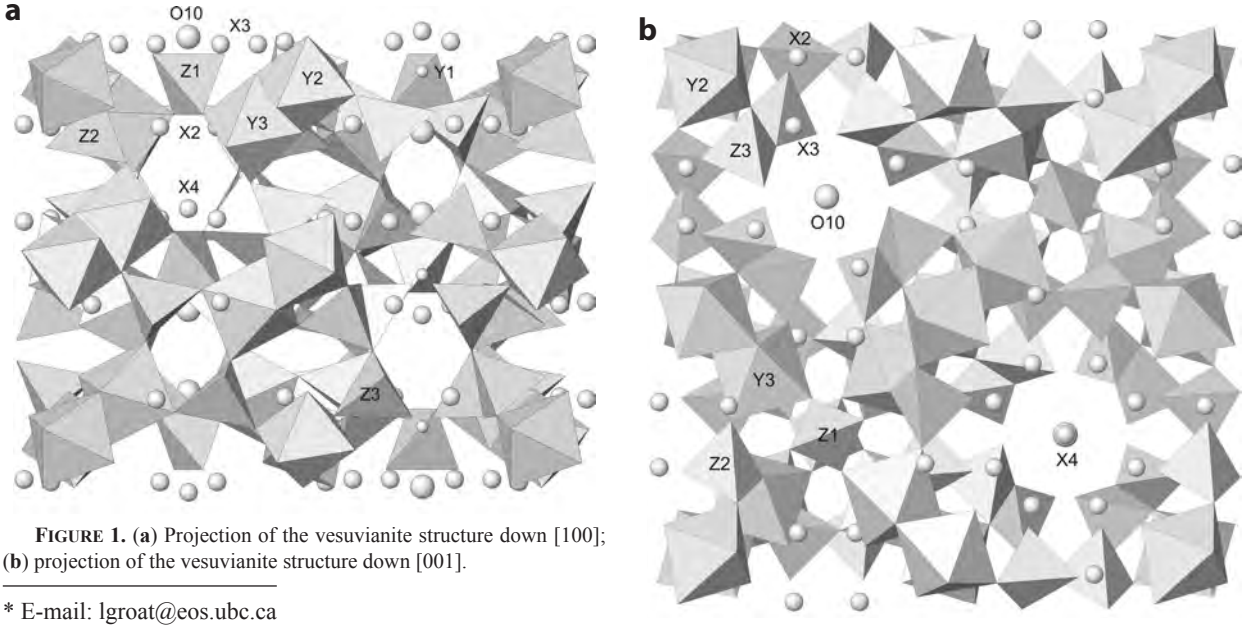

Figure 1. (**a**) Projection of the vesuvianite structure down [100]; (**b**) projection of the vesuvianite structure down [001].

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0003-004X/12/0010–1627$05.00/DOI: http://dx.doi.org/10.2138/am.2012.4091

adjacent channels may have X4 and Y1 at different *z* levels (e.g., Giuseppetti and Mazzi 1983; Fitzgerald et al. 1986; Allen and Burnham 1992; Pavese et al. 1998; Armbruster and Gnos 2000a, 2000b). The different X4 and Y1 arrangements lead to various tetragonal space goups. Allen and Burnham (1992) showed that ordered channel arrangements are favored in vesuvianites grown at <300 °C, and such crystals exhibit either *P*4/*n* or *P*4*nc* symmetry. In addition, a crystal might be assembled of domains representing both space groups, in which case the resulting space group becomes space group *P*4. Vesuvianite crystals grown at 400–800 °C exhibit disordered channel arrangements and the resulting symmetry is *P*4/*nnc* (Allen and Burnham 1992).

Flink (1886) was the first to describe deep red, Mn-bearing vesuvianite occurring in hausmannite ore from Långban in Sweden as granular aggregates and pods. Flink (1923) noted that it was mainly collected from the Norrbotten working. Groat et al. (1992a) reported up to 3.80 wt% MnO (1.61 Mn^{2+} per formula unit) and 2.49 wt% Bi_2O_3 (0.32 Bi apfu, atoms per formula unit) in bright-red crystals of vesuvianite from Långban.

Armbruster and Gnos (2000) described strongly zoned Mn-rich vesuvianite crystals with up to 14.3 wt% MnO from the N′chwaning II mine of the Kalahari manganese fields in the Republic of South Africa, where they formed by hydrothermal alteration of primary manganese ores below 450 °C. The studied crystals had either space group *P*4*nc* or *P*4/*n* due to partial long-range ordering, but most crystals were comprised of space group *P*4*nc* and *P*4/*n* domains yielding *P*4 average symmetry. The crystal structure of one crystal of average composition $Ca_{19}Mn_{3.5}Al_{9.5}Si_{17.4}(O,OH)_{78}$ was refined from single-crystal X-ray data in space group *P*4/*n*. The results showed that Mn^{2+} and Mn^{3+} are concentrated at the Y1 site, and additional Mn^{3+} is located at the Y2a (35%), Y1a (22%), Y2b (13%), and Y1b (8%) sites. Electron microprobe analyses and crystal-structure refinements indicated vacancies at the Z1 and Z2 sites, and structural and chemical evidence combined with the similarity of the structures of vesuvianite and garnet suggested a partial hydrogarnet-like substitution of SiO_4 tetrahedra by H_4O_4.

Armbruster et al. (2002) described the new mineral manganvesuvianite from the Wessels and N′Chwaning II mines in the Kalahari manganese fields. It was defined as a vesuvianite group mineral with Mn^{3+} occupying the Y1 position, and with simplified formula $Ca_{19}Mn^{3+}(Al,Mn^{3+},Fe^{3+})_{10}(Mg,Mn^{2+})_2Si_{18}O_{69}(OH)_9$.

We undertook this study to investigate the locations of Mn and Bi in the crystal structure of the red vesuvianite from Långban.

Experimental methods

Powder-diffraction data were collected at UBC with a Siemens D5000 diffractometer equipped with a diffracted-beam graphite monochromator and a Cu X-ray tube operated at 40 kV and 40 mA. Data were collected from 3 to 60° 2Θ with a scanning step of 0.02° 2Θ. The sample was also examined with a Philips XL30 scanning electron microscope (SEM) at the University of British Columbia, which is equipped with an energy-dispersion X-ray spectrometer (EDS).

Single-crystal X-ray diffraction measurements were made at C-HORSE (the Center for Higher Order Structure Elucidation, in the Department of Chemistry at UBC) using a Bruker X8 APEX II diffractometer with graphite monochromated Mo*K*α radiation. Data were collected in a series of φ and ω scans in 0.50° oscillations with 10.0 s exposures. The crystal-to-detector distance was 40 mm. Data were collected and integrated using the Bruker SAINT software package (Bruker 2007). Data were corrected for absorption effects using the multi-scan technique (SADABS, Sheldrick 1996) and were corrected for Lorentz and polarization effects.

All refinements were performed using the SHELXTL crystallographic software package (Sheldrick 2008) of Bruker AXS. Scattering factors for neutral atoms were used for the cations, and ionic factors from Azavant and Lichanot (1993) for O^{2-} were used for oxygen. The weighting scheme was based on counting statistics. Neutral atom scattering factors were taken from Cromer and Waber (1974). Anomalous dispersion effects were included in F_{calc} (Ibers and Hamilton 1964); the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley (1992). The values for the mass attenuation coefficients are those of Creagh and Hubbell (1992).

The crystal structures were initially refined in space group *P*4/*nnc* using parameters from the F-bearing vesuvianite V4 of Groat et al. (1992b) and the site nomenclature of Groat et al. (1992a). The structure of the vesuvianite II crystal (see below) was refined first and converged to an R_1 index of 0.0788 for an anisotropic displacement model. At this stage the atom at the Y1 site exhibited very large displacement parameters that were subsequently modeled by splitting the site into two half-occupied sites (Y1A and Y1B) constrained to have equal occupancies and equal isotropic displacements, as was done by Groat et al. (1992b) for F-bearing vesuvianite, Groat et al. (1994a) for vesuvianite with excess Y-group cations, and Groat et al. (1994b) for B-bearing vesuvianite (subsequently named wiluite; Groat et al. 1998). The atom at the O7 site also had very large displacement parameters that were modeled by splitting the site into two half-occupied sites constrained to have a combined total occupancy of 1.0 and to have equal isotropic displacements, as was done by Groat et al. (1994b, 1996) for boron-bearing vesuvianite.

At this point, difference Fourier maps showed significant residual density at the T1 position at 0.0565, 0.0565, ¼, (Wyckoff 8*h*). As suggested by bond-valence analysis (see below) As was placed at the T1 position. The difference-Fourier maps also showed significant residual density at the general position at 0.910, 0.837, 0.866 (Wyckoff 16*k*) and the special position at ¾, ¾, 0.831 (Wyckoff 4*e*). Bismuth was placed at the general position (henceforth labeled Bi3) and Cl at the special (Cl) position, and full-matrix least-squares refinement of all variable parameters converged to an R_1 index of 0.0170. No further peaks were observed in subsequent difference Fourier maps.

At this stage the site-scattering values for X1–4 and Y3 were allowed to vary freely. The results suggested limited substitution of a heavier cation at the X1, X2, and Y3 positions. Accordingly, Mn was refined against Ca at the X1 and X2 sites and against Al at the Y3 position. The final R_1 value was 0.0167.

The structure of the vesuvianite I crystal was refined in much the same way, except the Y1 site was not split and no Mn was evident at the X2 position. The merging *R* value was 0.1 (presumably a function of the unfavorable geometry of the sample, a 30 μm thick flake) and the final R_1 value was 0.0445. The merging *R* value for data from a second vesuvianite I crystal, also a 30 μm thick flake, collected over 24 h, was 0.09, and the final R_1 value was 0.0286. However, the refined Bi content of the second crystal was lower (0.43 vs. 0.56 Bi apfu), so the first refinement is presented here.

Data for the vesuvianite II crystal showed 14 systematic absence violations, three of which violate *P*4/*nnc*, *P*4/*n*, and *P*4*nc* symmetry. The remaining 11 reflections suggest *P*4/*n* symmetry, but they are very weak [maximum F_o^2 0.61(9), average 0.17(3)]. Refinement of the vesuvianite I structure in space group *P*4/*n* resulted in approximately the same R_1 value as the space group *P*4/*nnc* model, so the decision was made to retain the higher-symmetry space group. Data from nine other vesuvianite II crystals showed no more than two systematic absence violations per data set. Data for the vesuvianite I crystal showed no violating reflections at all.

According to Armbruster and Gnos (2000a), speculation that many vesuvianite crystals refined in space group *P*4/*nnc* are actually long-range ordered *P*4*nc* can be ruled out because the refinement results in a high-R_1 value. In addition, they noted that if the structure of a long-range ordered vesuvianite of true space group *P*4*nc* is erroneously refined in space group *P*4/*nnc*, then F_o^2 is always greater than F_c^2 in the list of most disagreeable reflections. This effect is especially pronounced for weak reflections, such as 147, 013, 057, 143, and 077. No such distribution was seen in the lists for our vesuvianite data.

Armbruster and Gnos (2000a) also describe another test where $F_c/F_c(\max)$ values are divided into 10 groups based on magnitude and a *K* value [where $K = \text{mean}(F_o^2)/\text{mean}(F_c^2)$] is determined for each group. An incorrect model or space group increases the *K* values of the weakest vesuvianite reflections up to a value of 10. In our refinements none of the *K* values were greater than 1.5.

Electron microprobe compositions were obtained with a fully automated CAMECA SX-50 microprobe operating in the wavelength-dispersion mode with the following operating conditions: excitation voltage, 20 kV; beam current, 40 nA; peak count time, 20 s (As 40 s, Cl 80 s, F 100 s); background count time, 10 s

(As 20 s, Cl 40 s, F 50 s); spot diameter, 5 µm. Data reduction was done using the "PAP" Φ(PZ) method (Pouchou and Pichoir 1991). For the elements considered, the following standards, X-ray lines and crystals were used: tennantite, As*Kα*, LIF; wollastonite, Si*Kα*, TAP; kyanite, Al*Kα*, TAP; synthetic fayalite, Fe*Kα*, LIF; bismuth element, Bi*Lα*, LIF; diopside, Mg*Kα*, TAP; wollastonite, Ca*Kα*, PET; synthetic rhodonite, Mn*Kα*, LIF; topaz, F*Kα*, TAP; and scapolite, Cl*Kα*, PET. Formulas were calculated from the electron microprobe data on the basis of 78 O and 9 (OH + F + Cl) atoms per formula unit.

Results

Examination of the sample described by Groat et al. (1992a) revealed small, rounded red crystals of vesuvianite with black Mn-oxide minerals and white calcite. X-ray powder diffraction data confirmed the presence of vesuvianite, hausmanite, and calcite. Subsequently, a polished thin section was created from this sample. Investigation with a petrographic microscope showed that the vesuvianite is a pale-pink color in plane-polarized light and examination of grain mounts (using a refractive index oil with n = 1.720) showed that the mineral is uniaxial negative. Investigation with the scanning electron microscope in backscattered electron imaging mode showed that very few of the vesuvianite crystals exhibit cores of higher average atomic number; these were labeled vesuvianite I, whereas the bulk or rims of the crystals were designated as vesuvianite II. The largest such core (Fig. 2) was subsequently removed from the polished thin section with a microscope-mounted drill (manufactured by U. Medenbach, Witten, Germany) and was attached to a glass fiber with epoxy for the single-crystal X-ray diffraction study. Several other crystals selected at random from the bulk sample were also used for the single-crystal X-ray diffraction study, and the results showed that all were vesuvianite II. After collection of X-ray diffraction data, all of the single crystals were attached to acrylic glass disks with epoxy and polished for the electron microprobe study. Examination with the scanning electron microscope showed no vesuvianite I cores in the vesuvianite II crystals used in the single-crystal X-ray diffraction study.

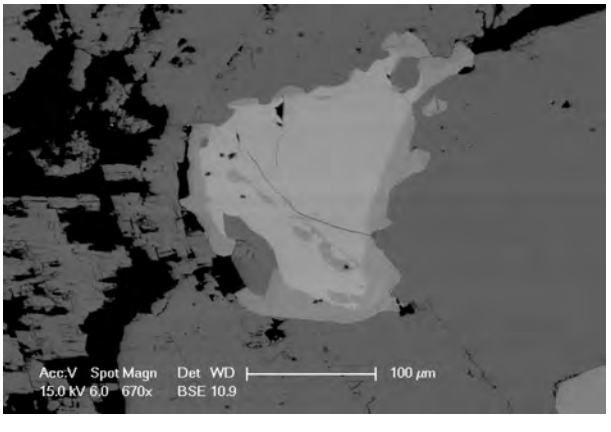

Figure 2. Backscattered-electron image of a vesuvianite crystal with a vesuvianite I core (subsequently extracted from the polished thin section and used for the single-crystal X-ray diffraction study) and a vesuvianite II rim.

Compositions

Average electron microprobe compositions are given in Table 1. The composition of the vesuvianite I crystal shows approximately the same amount of Mn (3.32 wt% MnO, or 1.43 Mn^{2+} apfu) and significantly more Bi (3.13 wt% Bi_2O_3, or 0.41 Bi^{3+} apfu) compared to the maximums reported by Groat et al. (1992a) for material from the same sample. The vesuvianite II composition shows considerably more Mn (4.14 wt% MnO, or 1.76 Mn^{2+} apfu) but less Bi (0.62 wt% Bi_2O_3, or 0.08 Bi^{3+} apfu) than the vesuvianite I composition. The vesuvianite I composition also shows considerably more Cl (0.82 wt% Cl, or 0.71 Cl apfu) than the vesuvianite II composition (0.13 wt% Cl, or 0.11 Cl apfu). The two compositions show similar smounts of As (0.56 wt% As_2O_5, or 0.15 As^{5+} apfu, and 0.62 wt% As_2O_5, or 0.16 As^{5+} apfu), which was not reported by Groat et al. (1992a).

Single-crystal X-ray diffraction studies

The refined unit-cell parameters were $a = 15.595$, $c = 11.779$ Å for the vesuvianite I crystal and $a = 15.585$, $c = 11.778$ Å for the vesuvianite II sample. These are similar to the values of $a = 15.592$, $c = 11.780$ Å reported by Groat et al. (1992a) for a red vesuvianite crystal from Långban. All of these unit-cell dimensions plot between the trends for boron-free and boron-bearing vesuvianite on the graph of *a* vs. *c* in Groat et al. (1992a), and between the fields defined for Mn-bearing vesuvianite (*P*4*nc* and *P*4/*n*) and wiluite (*P*4/*nnc*) on the graph of *a* vs. *c* in Gnos and Armbruster (2006).

Table 1. Average electron–microprobe compositions

	Vesuvianite I		Vesuvianite II	
n	3	σ	7	σ
As_2O_5	0.56	0.01	0.62	0.14
Sb_2O_5	0.09	0.00	0.09	0.00
SiO_2	35.43	0.04	36.10	0.27
Al_2O_3	14.27	0.22	14.39	0.27
Bi_2O_3	3.13	0.10	0.62	0.11
MgO	4.16	0.07	4.02	0.19
CaO	34.01	0.03	34.95	0.21
MnO	3.32	0.03	4.14	0.13
FeO	0.69	0.02	1.01	0.24
F	1.50	0.11	1.28	0.05
Cl	0.82	0.03	0.13	0.01
H_2O*	1.73	0.04	2.05	0.03
O=F	–0.63	0.05	–0.54	0.02
O=Cl	–0.19	0.00	–0.03	0.00
Total	98.95	0.91	98.90	0.48
As^{5+}	0.150	0.002	0.162	0.036
Sb^{5+}	0.017	0.000	0.018	0.003
Si^{4+}	18.056	0.031	18.096	0.065
Al^{3+}	8.571	0.048	8.499	0.126
Bi^{3+}	0.411	0.010	0.081	0.015
Mg^{2+}	3.158	0.027	3.006	0.147
Ca^{2+}	18.571	0.164	18.772	0.124
Mn^{2+}	1.433	0.004	1.756	0.061
Fe^{2+}	0.293	0.006	0.424	0.100
F^-	2.422	0.164	2.027	0.076
Cl^-	0.705	0.018	0.114	0.011
H^+	5.873	0.182	6.859	0.068
O^{2-}	74.873	0.182	75.859	0.068
Al + Mg	11.729		11.505	
Mn + Fe	1.726		2.180	

Notes: Compositions renormalized on 78 anions and 9 (OH + F + Cl). Na, P, Ti, Cu, Zn, Sn, and Pb were sought but not detected.

TABLE 2. Data measurement and refinement information

	Vesuvianite I	Vesuvianite II
a (Å)	15.595(1)	15.5852(9)
c (Å)	11.779(1)	11.7782(7)
V (Å^3)	2864.7(9)	2860.9(3)
Space group	*P4/nnc*	*P4/nnc*
Z	4	4
Crystal size (mm)	0.10 x 0.10 x 0.03	0.18 x 0.15 x 0.10
Radiation	Mo*K*α	Mo*K*α
Monochromator	graphite	graphite
Total F_o	16555	31775
Unique F_o	2108	2737
$F_o > 4\sigma F_o$	1145	2560
R_{int}	0.1(1)	0.019(9)
L.s. parameters	179	179
Range of *h*	−21 ≤ 18	−22 ≤ 23
Range of *k*	−21 ≤ 20	−23 ≤ 11
Range of *l*	−16 ≤ 12	−16 ≤ 18
R_1 for $F_o > 4\sigma F_o$	0.0445	0.0167
R_1 for all unique F_o	0.1358	0.0192
wR_2	0.1113	0.0464
a	0.0302	0.0164
b	7.37	2.27
GooF (=*S*)	1.030	1.206
$\Delta\rho_{max}$ (e Å^{-3})	1.23	1.09
$\Delta\rho_{min}$ (e Å^{-3})	−0.86	−0.30

Note: $w = 1/[s^2(F_o^2) + (a \times P)^2 + b \times P]$ where $P = [\text{Max}(F_o^2, 0) + 2 \times F_c^2)]/3$.

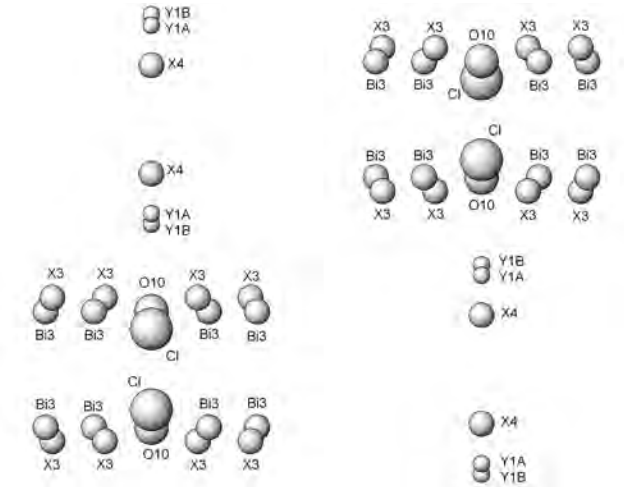

FIGURE 3. Details of the atomic positions in the channels in vesuvianite II (projected down [100]).

Crystal structure refinement

Data collection and refinement parameters for the single-crystal X-ray experiments are summarized in Table 2, positional and displacement parameters in Table 3, and bond lengths in Table 4. Complete crystal structure refinements for samples vesuvianite I and II are deposited as CIFs[1].

The atom at the X1 site is coordinated by eight O atoms: four at O1 positions (at distances of 2.330 Å in vesuvianite I and 2.3282 Å in vesuvianite II) and four at O2 sites (at distances of 2.514 and 2.5090 Å for vesuvianite I and II, respectively). The mean X1-O distance is 2.422 Å for vesuvianite I and 2.4186 Å for vesuvianite II. The refined site occupancy and bond distances indicate 0.904 Ca and 0.096 Mn^{2+} apfu at the X1 site in vesuvianite I and 0.880 Ca and 0.120 Mn^{2+} apfu at the X1 site in vesuvianite II.

The atom at the X2 site is coordinated by eight O atoms at distances of 2.332 to 2.998 Å (mean 2.474 Å) for vesuvianite I and 2.3294 to 3.015 Å (mean 2.476 Å) for vesuvianite II. The refined site occupancy and bond distances suggest only Ca at the X2 site in vesuvianite I and both Ca (0.961 apfu) and Mn^{2+} (0.039 apfu) at the X2 site in vesuvianite II.

The atom at the X3 position is coordinated by eight O atoms, three of which are at O7 sites. When the O7A sites are occupied, the mean X3-O distances are 2.50 and 2.497 Å for vesuvianite I and II, respectively, and when the O7B positions are occupied, the mean distances become 2.53 and 2.524 Å, respectively. The refined site occupancy suggests both Ca (0.88 apfu for vesuvianite I and 0.98 apfu for vesuvianite II) and vacancies (0.12 and 0.02 for vesuvianite I and vesuvianite II, respectively) at the X3 site.

The atom at the Bi3 position is also coordinated by eight O atoms or, given that the O10 and Cl sites (see below) are approximately equidistant from the Bi position, seven O atoms and one Cl atom. Three of the O atoms are at O7 positions. When the O7A sites are occupied the mean Bi3-O distances are 2.51 and 2.50 Å for vesuvianite I and II, respectively, and when the O7B positions are occupied the mean distances become 2.53 and 2.52 Å, respectively. The refined site occupancy and bond distances and valence suggest both Bi^{3+} (0.07 apfu in vesuvianite I and 0.015 apfu in vesuvianite II) and vacancies (0.93 apfu in vesuvianite I and 0.985 apfu in vesuvianite II) at the Bi3 position. The Bi3 position is 0.41 (vesuvianite I) and 0.44 (vesuvianite II) Å away from the X3 position (Fig. 3) and cannot be occupied when the X3 site is occupied.

The atom at the X4 site is coordinated by eight O atoms, four at O6 sites (at distances of 2.252 Å in vesuvianite I and 2.281 Å in vesuvianite II) and four at O9 positions (at distances of 2.654 and 2.617 Å for vesuvianite I and II, respectively), for mean X4-O distances of 2.453 (vesuvianite I) and 2.449 Å (vesuvianite II). The refined site occupancies of 1.032 apfu (vesuvianite I) and 1.010 apfu (vesuvianite II) suggest that in both crystals the X4 position is fully occupied by Ca.

In vesuvianite I, the Y1 position is coordinated by four O atoms at the O6 site and one O atom at the O10 site. The Y1-O6 distances are 2.051 Å and the Y1-O10 distance is 2.04 Å, for a mean Y1-O distance of 2.049 Å. Previous studies have suggested that Fe orders preferentially at the Y1 position; however, because the average electron microprobe composition shows only 0.293 Fe apfu for vesuvianite I, the Y1 site must be predominantly occupied by Mn, and the refined site occupancy with Mn at the Y1 position is 0.960 apfu. Bond-valence analysis suggests that the Mn, and presumably Fe, at the Y1 site in vesuvianite I is predominantly divalent.

In vesuvianite II, the Y1A-O6 distances are slightly shorter (2.047 Å) but the Y1A-O10 distance is significantly longer (2.287 Å), and the mean Y1A-O distance is 2.095 Å. Armbruster and Gnos (2000b) and Armbruster et al. (2002) showed that in Mn-rich vesuvianite Mn^{3+} preferentially occupies the Y1 site, and

[1] Deposit item AM-12-064, CIFs. Deposit items are available two ways: For a paper copy contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. For an electronic copy visit the MSA web site at http://www.minsocam.org, go to the *American Mineralogist* Contents, find the table of contents for the specific volume/issue wanted, and then click on the deposit link there.

TABLE 3. Positional and displacement parameters

Atom		Vesuvianite I	Vesuvianite II
X1	*x/a*	¾	¾
	y/b	¼	¼
	z/c	¼	¼
	U_{eq}	0.0127(6)	0.0105(1)
	population	0.226(6) Ca + 0.024 Mn	0.220(2) Ca +0.030 Mn
X2	*x/a*	0.81066(7)	0.81044(1)
	y/b	0.04548(7)	0.04569(1)
	z/c	0.37882(9)	0.37909(2)
	U_{eq}	0.0123(4)	0.00884(6)
	population	1.0 Ca	0.961(4) Ca + 0.039 Mn
X3	*x/a*	0.9023(4)	0.90003(5)
	y/b	0.8205(6)	0.82040(9)
	z/c	0.893(1)	0.8937(2)
	U_{eq}	0.0189(9)	0.0151(2)
	population	0.88(4) Ca	0.98(1) Ca
Bi3	*x/a*	0.911(1)	0.9100(8)
	y/b	0.836(1)	0.837(1)
	z/c	0.868(2)	0.866(1)
	U_{eq}	0.012(3)	0.010(2)
	population	0.07(1) Bi	0.015(2) Bi
X4	*x/a*	¾	¾
	y/b	¾	¾
	z/c	0.1369(6)	0.14124(8)
	U_{eq}	0.014(2)	0.0116(3)
	population	0.129(3)	0.1262(7)
Y1A	*x/a*	¾	¾
	y/b	¾	¾
	z/c	0.0568(5)	0.0611(2)
	U_{eq}	0.016(1)	0.0076(3)
	population	0.120(2) Mn	0.0557(3) Mn
Y1B	*x/a*	–	¾
	y/b	–	¾
	z/c	–	0.0402(2)
	U_{eq}	–	0.0076(3)
	population	–	0.0557(3) Fe
Y2	*x/a*	0	0
	y/b	0	0
	z/c	0	0
	U_{eq}	0.0100(5)	0.00788(9)
Y3	*x/a*	0.88771(9)	0.88896(2)
	y/b	0.12017(9)	0.12004(2)
	z/c	0.1260(1)	0.12631(3)
	U_{eq}	0.0104(4)	0.0079(1)
	population	0.940(6) Al + 0.060 Mn	0.909(2) Al + 0.091(2) Mn
Z1	*x/a*	¼	¼
	y/b	¾	¾
	z/c	0	0
	U_{eq}	0.0087(6)	0.0069(1)
Z2	*x/a*	0.82001(8)	0.82021(2)
	y/b	0.04132(8)	0.04095(2)
	z/c	0.8711(1)	0.87104(2)
	U_{eq}	0.0073(3)	0.00628(6)
Z3	*x/a*	0.91633(9)	0.91611(2)
	y/b	0.84938(9)	0.84959(2)
	z/c	0.3641(1)	0.36419(3)
	*U*eq	0.0115(3)	0.00809(7)
T1	*x/a*	0.056(2)	0.0565(2)
	y/b	0.056(2)	0.0565(2)
	z/c	¼	¼
	U_{eq}	0.05(1)	0.010(1)
	population	0.020(2) As	0.0167(5) As
O1	*x/a*	0.7797(2)	0.78047(5)
	y/b	0.1730(2)	0.17284(5)
	z/c	0.0852(3)	0.08561(7)
	U_{eq}	0.0124(8)	0.0098(2)
O2	*x/a*	0.8819(2)	0.88172(5)
	y/b	0.1603(2)	0.16035(5)
	z/c	0.2809(3)	0.28043(7)
	U_{eq}	0.0106(8)	0.0097(1)
O3	*x/a*	0.9541(2)	0.95478(6)
	y/b	0.2234(2)	0.22343(5)
	z/c	0.0756(3)	0.07585(7)
	U_{eq}	0.0114(8)	0.0105(2)
O4	*x/a*	0.9391(2)	0.93917(5)
	y/b	0.1055(2)	0.10559(5)
	z/c	0.4693(3)	0.46983(7)
	U_{eq}	0.0111(8)	0.0087(1)
O5	*x/a*	0.8284(2)	0.82863(5)
	y/b	0.0125(2)	0.01285(6)
	z/c	0.1793(3)	0.17928(7)
	U_{eq}	0.0141(9)	0.0118(2)
O6	*x/a*	0.8794(2)	0.87897(7)
	y/b	0.7264(2)	0.72567(6)
	z/c	0.0581(3)	0.05563(8)
	U_{eq}	0.0192(9)	0.0158(2)
O7A	*x/a*	0.823(2)	0.8233(3)
	y/b	0.9435(7)	0.9437(1)
	z/c	0.822(1)	0.8213(2)
	U_{eq}	0.011(1)	0.0093(2)
	population	0.61(9) O	0.56(1) O
O7B	*x/a*	0.841(2)	0.8421(3)
	y/b	0.949(1)	0.9476(2)
	z/c	0.812(2)	0.8110(3)
	U_{eq}	0.011(1)	0.0093(2)
	population	0.39(9) O	0.44(1) O
O8	*x/a*	0.9394(2)	0.93986(5)
	y/b	0.9084(2)	0.90809(5)
	z/c	0.0682(3)	0.06794(7)
	*U*eq	0.0105(8)	0.0087(1)
O9	*x/a*	0.8541(2)	0.85352(5)
	y/b	0.8541(2)	0.85352(5)
	z/c	¼	¼
	U_{eq}	0.013(1)	0.0117(2)
O10	*x/a*	¾	¾
	y/b	¾	¾
	z/c	0.883(4)	0.8669(5)
	U_{eq}	0.021(5)	0.0183(6)
	population	0.16(2) O	0.252(5) O
Cl	*x/a*	¾	¾
	y/b	¾	¾
	z/c	0.844(2)	0.831(2)
	U_{eq}	0.026(5)	0.021(5)
	population	0.10(1) Cl	0.016(3) Cl
O11	*x/a*	0.9967(2)	0.99715(5)
	y/b	0.0608(2)	0.06086(5)
	z/c	0.1364(3)	0.13716(7)
	U_{eq}	0.0100(7)	0.0091(2)

Armbruster et al. (2002) noted that this leads to a characteristic Jahn-Teller distortion for the Y1A site (*P*4/*n* model) with four Mn^{3+}-O distances of 1.975 Å and one of 2.125 Å. Although our Y1A-O distances are longer than the equivalent distances in Armbruster et al. (2002), the similar distortion suggests at least some Mn^{3+} at the Y1A position. However, the results of the bond-valence analysis (2.261 v.u.) indicates that most of the Mn is divalent.

Also in vesuvianite II, the Y1B-O6 and Y1B-O10 distances are 2.054 and 2.041 Å, respectively, for a mean Y1B-O distance of 2.051 Å. The average electron microprobe composition for vesuvianite II shows 0.424 Fe apfu, approximately enough to fill the Y1B position. The refined site occupancies of the Y1 positions in both crystals suggest minor vacancies (0.040 for vesuvianite I and a combined 0.109 for vesuvianite II).

The atom at the Y2 site is coordinated by O atoms at two O4, two O8, and two O11 positions, and the mean Y2-O distances are 1.897 and 1.8986 Å for vesuvianite I and II, respectively. The refined bond distances, bond valences, and site occupancy suggest that in both structures this site is completely occupied by aluminum.

The atom at the Y3 position is coordinated by six O atoms at

TABLE 4. Selected interatomic distances (Å)

		vesuvianite I	vesuvianite II
X1-O1	x4	2.330(4)	2.3282(8)
X1-O2	x4	2.514(3)	2.5090(8)
<X1-O>		2.422	2.4186
X2-O8a		2.334(4)	2.3294(8)
X2-O5b		2.332(4)	2.3306(9)
X2-O3c		2.378(4)	2.3769(9)
X2-O2		2.402(4)	2.4038(8)
X2-O5		2.422(4)	2.4250(9)
X2-O4		2.454(4)	2.4575(9)
X2-O1b		2.474(4)	2.4713(9)
X2-O6a		2.998(4)	3.015(1)
<X2-O>		2.474	2.476
X3-O7B		2.42(2)	2.386(3)
X3-O3d		2.370(7)	2.391(1)
X3-O7A		2.43(1)	2.418(3)
X3-O6e		2.46(1)	2.434(3)
X3-O11d		2.46(1)	2.475(2)
X3-O7Af		2.48(3)	2.492(5)
X3-O8e		2.539(8)	2.543(1)
X3-O7Bg		2.55(2)	2.544(4)
X3-O10		2.620(8)	2.602(1)
X3-O7Ag		2.62(2)	2.621(3)
X3-O7Bf		2.79(4)	2.813(6)
<X3-O,O7A>		2.50	2.497
<X3-O,O7B>		2.53	2.524
X3-Cl		2.681(9)	2.686(7)
Bi3-O7B		2.17(2)	2.13(1)
Bi3-O11d		2.16(2)	2.15(2)
Bi3-O7Bg		2.21(3)	2.16(2)
Bi3-O7A		2.23(2)	2.21(1)
Bi3-O7Ag		2.31(2)	2.27(1)
Bi3-O3d		2.40(1)	2.407(6)
Bi3-O7Af		2.60(3)	2.60(1)
Bi3-O8e		2.65(2)	2.668(6)
Bi3-Cl		2.86(2)	2.87(2)
Bi3-O6e		2.86(3)	2.86(2)
Bi3-O7Bf		2.90(4)	2.92(1)
<Bi3-O,Cl,O7A>		2.51	2.50
<Bi3-O,Cl,O7B>		2.53	2.52
X3-Bi3		0.41(2)	0.44(2)
Bi3-O10		2.85(2)	2.84(2)
X4-O6	x4	2.252(4)	2.281(1)
X4-O9	x4	2.654(5)	2.617(1)
<X4-O>		2.453	2.449

TABLE 4.—*CONTINUED*

		vesuvianite I	vesuvianite II
Y1A-O6	x4	2.051(4)	2.047(1)
Y1A-O10h		2.04(4)	2.287(6)
<Y1A-O>		2.049	2.095
Y1B-O10h		-	2.041(6)
Y1B-O6i	x4	-	2.054(1)
<Y1B-O>			2.051
Y2-O11j	x2	1.866(3)	1.8739(8)
Y2-O8k	x2	1.892(3)	1.8896(8)
Y2-O4l	x2	1.934(3)	1.9322(8)
<Y2-O>		1.897	1.8986
Y3-O2		1.931(4)	1.9242(9)
Y3-O11		1.939(4)	1.9262(9)
Y3-O1		1.935(4)	1.9405(9)
Y3-O3		2.003(4)	2.0006(9)
Y3-O5		2.017(4)	2.016(1)
Y3-O4m		2.067(4)	2.0629(9)
<Y3-O>		1.982	1.978
Z1-O1n	x4	1.632(3)	1.6397(8)
Z2-O7Ao		1.632(9)	1.627(2)
Z2-O3p		1.634(4)	1.6342(9)
Z2-O2c		1.631(4)	1.6381(9)
Z2-O7Bo		1.63(1)	1.653(3)
Z2-O4c		1.668(4)	1.6695(9)
<Z2-O,O7A>		1.641	1.642
<Z2-O,O7B>		1.64	1.649
Z3-O6q		1.603(4)	1.6134(9)
Z3-O8r		1.620(4)	1.6229(9)
Z3-O5s		1.618(4)	1.6255(9)
Z3-O9		1.659(2)	1.6626(6)
<Z3-O>		1.625	1.6311
T1-O11t	x2	1.62(1)	1.621(2)
T1-O7Bm	x2	1.78(5)	1.737(7)
<T1-O>		1.70	1.679
O10-Cl		0.46(2)	0.42(2)

Note: a: $y,x-1,-z+\frac{1}{2}$; b: $-x+\frac{1}{2},y,-z+\frac{1}{2}$; c: $-y+1,-x+1,z+\frac{1}{2}$; d: $-x+1,-y+1,-z+1$; e: $-x+1,y-\frac{1}{2},z-\frac{1}{2}$; f: $y-\frac{1}{2},-x+1,-z+1$; g: $x,-y+3/2,-z+3/2$; h: $x,y,z-1$; i: $-y+3/2,x-1,z$; j: $x,y,z+1$; k: $-x+1,-y+1,-z$; l: $-y,-x+1,z-\frac{1}{2}$; m: $-y+1,x+1,z-\frac{1}{2}$; n: $-y+\frac{1}{2},x,z$; o: $x-1,y,z$; p: $-y+1,x-\frac{1}{2},-z+1$; q: $-x+1,-y,-z$; r: $y,x,-z+\frac{1}{2}$; s: $y+1,x,-z+\frac{1}{2}$; t: $-y+3/2,-x+3/2,-z+3/2$.

distances of 1.931 to 2.067 Å in vesuvianite I (mean 1.982 Å) and 1.9242 to 2.0628 Å (mean 1.978 Å) in vesuvianite II. The refined site occupancy suggests 0.940 apfu (Al + Mg) and 0.060 apfu Mn at the Y3 site in vesuvianite I, and 0.909 apfu (Al + Mg) and 0.091 apfu Mn in vesuvianite II. Bond-valence analysis suggests that the Mn at the Y3 site is trivalent.

The atom at the Z1 site is coordinated by four O atoms at the O1 site at distances of 1.632 Å in vesuvianite I and 1.6397 Å in vesuvianite II. The bond distances and valences and refined site occupancies suggest that the Z1 position is fully occupied by Si in both structures.

The atom at the Z2 site is coordinated by four O atoms at the O7, O3, O2, and O4 sites. In vesuvianite I, the mean Z2-O distances are 1.641 (O7A occupied) and 1.64 Å (O7B occupied); for vesuvianite II, the corresponding Z2-O distances are 1.642 and 1.649 Å, respectively. The bond distances and valences and refined site occupancy suggest that the Z2 site is occupied by silicon.

The atom at the Z3 site is coordinated by four O atoms at the O6, O8, O5, and O9 positions, for mean Z3-O distances of 1.625 Å for vesuvianite I and 1.6311 Å for vesuvianite II. The bond distances and valences and refined site occupancy suggest that the Z3 position is fully occupied by silicon. We note that refinement of the occupancies of the *Z* sites showed no evidence of the partial hydrogarnet-like substitution of SiO_4 tetrahedra by H_4O_4 described by Armbruster and Gnos (2000b).

The atom at the T1 site is coordinated by two atoms at the O11 site (1.62 and 1.621 Å for vesuvianite I and II, respectively) and two atoms at the O7B sites (1.78 Å for vesuvianite I and 1.737 Å for vesuvianite II) for mean T1-O distances of 1.70 and 1.679 Å. These distances and the bond valences suggest that the T1 site contains As; the refined site occupancies are 0.040 apfu for vesuvianite I and 0.033 apfu for vesuvianite II.

For vesuvianite I the refined site occupancies of the O7A and O7B sites are 0.61 and 0.39, respectively, and the values for vesuvianite II are 0.56 and 0.44. The O7A-O7B distance is 0.31 Å in VI and 0.32 Å in VII, which is significantly shorter than the O7A-O7B distances of ~0.5 Å reported by Groat et al.

(1994, 1996) for boron-bearing vesuvianite.

In vesuvianite I, the atom at the O10 position (with occupancy 0.16) is 2.04 Å from the Y1 site, 2.620 Å from four X3 positions, and 2.85 Å from four Bi sites. In vesuvianite II, the atom at the O10 site is 2.041 Å from the Y1B position, 2.287 Å from the Y1A site, 2.602 Å from four X3 positions, and 2.84 Å from four Bi sites. The refined site occupancy of the O10 position is 1.008 apfu.

In vesuvianite I, the atom at the Cl site (occupancy 0.04) is 0.46 Å from the O10 position (Fig. 3), which suggests that they cannot both be occupied at the same time. The atom is also 2.681 Å from four X3 sites and 2.86 Å from four Bi3 positions. In the vesuvianite II crystal the atom at the Cl site is 0.42 Å from the O10 position, 2.686 Å from four X3 sites, and 2.87 Å from four Bi3 positions. The refined site occupancy of the Cl position is 0.064 apfu.

Discussion

The average electron microprobe compositions and the compositions from the site refinements result in the following formulas for vesuvianite I:

$Ca_{18.57}Bi_{0.41}(Mn_{1.43}Fe_{0.29})_{\Sigma 1.72}(Al_{8.57}Mg_{3.16})_{\Sigma 11.73}(As_{0.15}Sb_{0.02})_{\Sigma 0.17}Si_{18.06}(O_{69}OH_{5.87}F_{2.42})_{\Sigma 77.29}Cl_{0.71}$ (electron microprobe analysis, EMPA);

$Ca_{17.88}Bi_{0.56}(Mn,Fe)_{\Sigma 1.63}(Al,Mg)_{\Sigma 11.52}(As,Sb)_{\Sigma 0.16}Si_{18.00}(O,OH,F)_{\Sigma 77.28}Cl_{0.80}$ (SREF).

And for vesuvianite II:

$Ca_{18.77}Bi_{0.08}(Mn_{1.76}Fe_{0.42})_{\Sigma 2.18}(Al_{8.50}Mg_{3.01})_{\Sigma 11.51}(As_{0.16}Sb_{0.02})_{\Sigma 0.18}Si_{18.10}(O_{69}OH_{6.86}F_{2.03})_{\Sigma 77.89}Cl_{0.11}$ (EMPA);

$Ca_{18.23}Bi_{0.12}(Mn,Fe)_{\Sigma 2.17}(Al,Mg)_{\Sigma 11.52}(As,Sb)_{\Sigma 0.16}Si_{18.00}(O,OH,F)_{\Sigma 78.02}Cl_{0.13}$ (SREF).

Although the formulas are similar, Ca is notably higher in the electron microprobe compositions. This might result from poor standards or problems with the data reduction method. In addition, Ca is the most abundant cation and would be highly affected by the assumptions made when renormalizing the electron microprobe compositions.

The results show Mn at the X1 (0.19 Mn^{2+} apfu), Y1 (0.71 Mn^{2+} apfu, assuming a fully occupied Y1 site with 0.29 Fe^{2+} from EMPA), and Y3 (0.48 Mn^{3+} apfu, assuming no Fe at Y3) positions in vesuvianite I, for totals of 0.90 Mn^{2+} apfu and 0.48 Mn^{3+} apfu. For vesuvianite II the results show Mn at the X1 (0.24 Mn^{2+} apfu), X2 (0.31 Mn^{2+} apfu), Y1A (0.45 Mn^{2+} apfu), and Y3 (0.73 Mn^{3+} apfu, assuming no Fe at Y3) sites for totals of 0.90 Mn^{2+} and 0.45 Mn^{3+} apfu.

Are these manganvesuvianites? Armbruster et al. (2002) defined manganvesuvianite as a vesuvianite-group mineral where the Y1 position is occupied by Mn^{3+}. Our results show that Mn dominates the Y1 site in vesuvianite I and, if it is trivalent, the sample fits the definition of managanvesuvianite. However, the bond valence analysis suggests that the Mn is divalent, in which case vesuvianite I would potentially be a new mineral, although it is difficult to define a new species based on a valence change unless it results in a change in anions (J. Grice, pers. comm.). The situation is even less clear for vesuvianite II, where the results suggest that the Y1A site contains Mn and the Y1B position is occupied by iron. Since the occupancies of the two sites are constrained to be the same, Mn would occupy 50% of an unsplit Y1 site, and if the Mn is trivalent the crystal would be halfway between vesuvianite and manganvesuvianite. However the bond-valence analysis suggests that the Mn is divalent, so presumably the sample is halfway between vesuvianite and the potential new species.

The results also show 0.56 (vesuvianite I) and 0.12 (vesuvianite II) Bi^{3+} apfu at the new Bi3 position. The Bi3 site is 0.41 (vesuvianite I) and 0.44 Å (vesuvianite II) from the X3 position, which is necessarily vacant when Bi3 is occupied (and vice versa). The atoms at the Bi3 and X3 sites have almost the same coordination sphere, although some of the bond distances differ by as much as ~0.3 Å (Table 4), and their similar occupancies suggest that the Bi atom may be bonding to the Cl atom at the Cl site instead of the atom at the O10 position; however, the Bi3-Cl and Bi3-O10 distances are about the same.

The results show 0.16 (vesuvianite I) and 0.13 (vesuvianite II) As^{5+} apfu (and presumably minor Sb, from the electron microprobe compositions) at the T1 position. Groat et al. (1994a) showed that the T1 position in vesuvianite crystals with excess Y-group cations is occupied by (Al,Fe), which replaces two H atoms at adjacent H1 positions. Local bond-valence arguments showed that the substitution is accompanied by the incorporation of a vacancy at an adjacent X3 site. Our site-refinement results show the combined occupancies of the X3, Bi3, and T1 positions is approximately one, which would support this argument.

When occupied, the atom at the T1 position is coordinated by O atoms at two O7B sites and presumably O atoms (for charge balance) at two O11 positions. However the occupancy of the O7B site (0.39 in vesuvianite I, and 0.44 in vesuvianite II) is much greater than that of the T1 position due most likely to F for OH substitution at the neighboring O11 position. Groat et al. (1992b) showed that F substitutes for OH at both the O10 and OH (=O11) sites in the crystal structure, but that the former can only occur to a maximum of 1 F apfu and results in significant positional disorder involving both the anions at the O10 position and the cations at the coordinating Y3 position. Since our EMPA show more than 1 F apfu, and there is no evidence for significant positional disorder at O10 or Y3, we suggest that the O11 site contains OH and F when T1 is vacant.

Previous studies (Yoshiasa and Matsumoto 1986; Groat et al. 1992b) have shown that when O11 contains OH there is a strong hydrogen bond between the H atom at the H1 site and the O atoms at two neighboring O7 positions. Groat et al. (1992b) showed that increased F for OH substitution at O11 leads to an aggregate shortening of O7-X3 bond distances. In vesuvianite I and II, F occupancies at O11 of 0.30 and 0.25, respectively corresponds to the loss of twice as many H bonds to O atoms at O7 positions, and hence to the observed O7A occupancies of 0.61 and 0.56.

The local environment of the Cl position and related interatomic distances are similar in samples vesuvianite I and II. In the vesuvianite II sample, the Cl atom at the Cl position is 0.42

Å from the O10 site and 1.91 Å from a symmetry-equivalent Cl position. It is also 2.46 Å from a Y1b site, 2.686 Å from four X3 positions, 2.71 Å from a Y1A site, and 2.87 Å from four Bi3 positions. All of these Cl to cation distances are longer than the equivalent cation to O10 distances, except those to Bi3, which are approximately equivalent. This and their similar occupancies suggest that the Cl atom at the Cl site is bonded to the Bi atom at the Bi3 position when it is occupied, and that when this happens there is a vacancy at the O10 position.

It is obvious that at Långban, the vesuvianite I crystals formed first and that the much more common vesuvianite II crystals are younger and in some cases form rims on vesuvianite I cores. Relative to vesuvianite I, the vesuvianite II crystals contain more Mn and Fe, but less Bi, Mg, and Cl, suggesting that the parental fluid had a slightly different composition. Their *P*4/*nnc* symmetry indicates that both vesuvianite crystals formed at high temperatures (400–800 °C), although the few violating reflections in the vesuvianite II crystal suggest that it formed at a lower temperature approaching those where ordered channel arrangements are favored.

Acknowledgments

The authors thank J. Engelbrecht for helping prepare the manuscript, which was improved by comments from M. Parker, J. Grice, an anonymous reviewer, and Associate Editor A. Celestian. Financial support was provided by the Natural Sciences and Engineering Research Council of Canada in the form of a Discovery Grant to L.A.G.

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Manuscript received January 2, 2012
Manuscript accepted May 25, 2012
Manuscript handled by Aaron Celestian

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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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O5 X2CA Y3AL 36.86(2) 5_655 5_655 ?
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