Uvite, CaMg₃(Al₅Mg)(Si₆O₁₈)(BO₃)₃(OH)₃(OH), a new, but long-anticipated mineral species of the tourmaline supergroup from San Piero in Campo, Elba Island, Italy

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Abstract

Uvite, CaMg₃(Al₅Mg)(Si₆O₁₈)(BO₃)₃(OH)₃(OH), is a new mineral of the tourmaline supergroup. It occurs in the Facciatoia quarry, San Piero in Campo, Elba Island, Italy (42°45’04.55”N, 10°12’50.89”E) at the centre of a narrow (2–3 cm wide) vein composed of aggregates of dark brown to black tourmaline, penetrating (magnesite + dolomite)-rich hydrothermally altered metaserpentinite. Crystals are euhedral and up to 1 cm in size, brown with a vitreous lustre, conchoidal fracture and grey streak. Uvite has a Mohs hardness of 7½, a calculated density of 3.115 g/cm³ and is uniaxial (–). Uvite has trigonal symmetry, space group R₃m, a = 15.9519(10) Å, c = 7.2222(5) Å, V = 1597.3(1) Å³ and Z = 3. The crystal structure was refined to R₁ = 1.77% using 1666 unique reflections collected with MoKα X-rays. Crystal-chemical analysis resulted in the empirical crystal-chemical formula \( \frac{1}{2} \left( \text{Si}_{52} \text{Al}_{58} \text{Na}_{0.35} \text{O}_{18.00} \right) \left( \text{BO}_{3} \right)_{3}^{0.86} \left( \text{OH} \right)_{2.02} \left( \text{OH} \right)_{3.00} \) which recast in its ordered form for classification purposes is:

\[
\begin{align*}
X(\text{Ca}_{2.61} \text{Na}_{0.00} \text{Mg}_{1.00} \text{Si}_{2.00} \text{O}_{18.00}) & = 1 \times 10^{-5} \text{cm}^3 \\
Z(\text{Al}_{3.25} \text{Fe}^{3+}_{0.75} \text{Fe}^{2+}_{0.25} \text{Si}_{12.00} \text{O}_{18.00}) & = 1 \times 10^{-5} \text{cm}^3
\end{align*}
\]

Uvite is a hydroxy-species belonging to the calcic-group of the tourmaline supergroup. The closest end-member compositions of valid tourmaline species are fluor-tourmaline and feruiterite, to which uvite is related by the substitutions \( W(\text{OH}) \leftrightarrow W^2F^- \) and \( Z(\text{Mg}^{2+}) \leftrightarrow Z(\text{Fe}^{2+}) \), respectively. The occurrence of a solid-solution between uvite and magnesio-lucenite, according to the substitution \( 2\text{Z} \text{Mg}^{2+} + \text{W}(\text{OH}) \leftrightarrow 2\text{Al}^{3+} + 2\text{W}^2\text{O}^4^- \), is supported by experimental data. The new mineral was approved by the IMA-CNMMNC (IMA 2019-113). Uvite from Facciatoia formed by the reaction between B-rich fluids, released during the crystallisation process of LCT pegmatites, and the surrounding metaserpentinites, altered by contact metamorphism in the aureole of the Miocene Mt. Capanne monzogranitic pluton.

Keywords: uvite, new mineral species, tourmaline, crystal-structure refinement, electron microprobe, Mössbauer spectroscopy, infrared spectroscopy, optical absorption spectroscopy

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Introduction

Tourmalines are complex borosilicates that have been studied extensively in terms of their crystal structure and crystal chemistry (e.g. Foit, 1989; Hawthorne, 1996; Hawthorne and Henry, 1999; Ertl et al., 2002; Novák et al., 2004; Bosi, 2013, 2018; Henry and Dutrow, 2011; Cempírek et al., 2013; Bačík and Fridrichová, 2021). In accordance with Henry et al. (2011), the...
general chemical formula of tourmaline is written as: $\text{XY}_2\text{Zr}_2\text{O}_{12}(\text{BO}_3)\text{V}_2\text{W}$, where $X = \text{Na}^+$, $\text{K}^+$, $\text{Ca}^{2+}$, $\square$ (= vacancy); $Y = \text{Al}^{3+}$, $\text{Fe}^{3+}$, $\text{Cr}^{3+}$, $\text{V}^{3+}$, $\text{Mg}^{2+}$, $\text{Fe}^{2+}$, $\text{Mn}^{2+}$, $\text{Li}$; $Z = \text{Al}^{3+}$, $\text{Fe}^{3+}$, $\text{Cr}^{3+}$, $\text{V}^{3+}$, $\text{Mg}^{2+}$, $\text{Fe}^{2+}$; $T = \text{Si}^{4+}$, $\text{Al}^{3+}$, $\text{B}^{3+}$; $B = \text{B}^{3+}$; $V = (\text{OH})$, $\text{O}^2$; and $W = (\text{OH})^-$, $\text{F}$, $\text{O}^2$. Note that the letters $X$, $Y$, $T$ and $Z$ and $B$ represent groups of cations at the $[9]$-$[6]$, $[4]$-$[3]$ and $[3]$-$[B]$ crystallographic sites (designated by italicised letters). The letters $V$ and $W$ in the formula represent groups of anions accommodated at the $[3]$-coordinated $O(3)$ and $O(1)$ crystallographic sites, respectively. The dominance of specific ions at one or more sites of the structure gives rise to numerous distinct mineral species.

A formal description of the new tourmaline species uvite is presented here. Uvite is a common mineral name in the tourmaline literature and refers to the province of Uva (Sri Lanka) as the type locality for the formerly supposed occurrence of this mineral (Kunitz, 1929). However, the tourmaline from the Uva locality should actually correspond to a fluor-species (Dunn et al., 1977). In accord with the tourmaline nomenclature scheme, the root name of fluor-uvite (Henry et al., 2011) requires that the name uvite should be given to the hydroxy analogue. The approval of this new species has been beset by difficulties. Uvite was approved by the International Mineralogical Association’s Commission on New Minerals, Nomenclature and Classification (IMA–CNMNC) as a valid mineral species with the proposal no. 2000-030a (Clark et al., 2010), but the complete description has never been published. This proposal was subsequently withdrawn as additional analytical work done by the authors of proposal 2000-30a showed this material to be a potentially new oxy-tourmaline (Hälenius et al., 2018). In July 2019, another proposal (no. 2019-004) was rejected. Finally, uvite has been approved by the IMA–CNMNC with proposal no. 2019-113 (Bosi et al., 2020) using a specimen collected at Facciatoia, at the eastern limit of the village of San Piero in Campo, Elba Island, in an abandoned magnesite quarry in 2019 by the mineral collector Michele Degl’Innocenti. Holotype material is deposited in the collections of the Natural History Museum of Milano, Italy, catalogue number M38848, and the Museo di Storia Naturale, University of Pisa, catalogue number 19911.

**Occurrence**

The holotype specimen was collected from a narrow vein of aggregates of dark brown-to-black tourmaline, penetrating hydrothermally altered metaserpentinite rich in magnesite and dolomite, in the abandoned Facciatoia quarry, east of the village of San Piero in Campo, Elba Island, Livorno, Tuscany, Italy (42°45’04.55”N, 10°12’50.89”E). Facciatoia is a classic mineralogical locality, in which several narrow LCT pegmatites rich in multicoloured and pink elbaite crystals were found in the past (today the locality is exhausted; Pezzotta, 2021); the pegmatites crosscut a lens of porphyritic monzogranite and the surrounding hydrothermally altered metaserpentinites.

In San Piero in Campo, tourmaline-rich veins typically cross-cut metaserpentinites around miarolitic tourmaline-bearing pegmatites in the metamorphic aureole of the Monte Cananno intrusion. These veins are up to 2 or 3 cm wide and can be up to a few metres long. They are entirely composed of tourmaline-supergroup minerals (uvite and magnesio-lucchesiite), and locally form small cavities in which tourmaline occurs as blackish sharp and lustrous short prisms, up to 1 cm long and 5 mm in diameter.

**Appearance, physical and optical properties**

Uvite occurs as massive vein-filling subhedral grains and rare euhedral crystals up to 1 cm in size and is brown with a vitreous lustre (Fig. 1). The morphology consists of {1010} and {1120} prisms terminated by {1011} and {1011} pyramidal faces. Prism faces are striated parallel to the c axis. It has a grey streak and shows no fluorescence, has a Mohs hardness of ~7½ (estimated by analogy with magnesio-lucchesiite; Scribner et al., 2021) and is brittle with a conchoidal fracture. The calculated density, based on the empirical formula and unit-cell volume refined from single-crystal X-ray diffraction (XRD) data, is 3.115 g/cm³. In thin section, uvite is transparent; in transmitted light, it is pleochroic, O = greenish brown, E = pale yellow, with $O > E$. Uvite is uniaxial (−) with refractive indices $\omega = 1.660(5)$ and $\varepsilon = 1.640(5)$ measured by the immersion method using white light from a tungsten source. The mean index of refraction, density, and chemical composition resulted in an excellent compatibility index ($1 - \text{Kp/Kc} = 0.021$) (Mandarino, 1981).

**Analytical methods and results**

**Microprobe analysis**

Electron microprobe analysis was done using a wavelength-dispersive spectrometer (WDS mode) with a Cameca SX50 instrument at the ‘Istituto di Geologia Ambientale e Geingegneria, CNR (Rome, Italy), operating at an accelerating potential of 15 kV, a sample current of 15 nA and 10 μm beam diameter. The following standards, X-ray Kz lines and analyser crystals were used: wollastonite (Si and Ca; TAP), magnetite (Fe; LIF), rutile (Ti; TET), corundum (Al; TAP), vanadinite (V; PET), fluorophlogopite (F; TAP), periclase (Mg; TAP), jadeite (Na; TAP), orthoclase (K; TET), sphalerite (Zn; LIF), chromium oxide (Cr; PET), and metallic Mn (Mn; LIF). The PAP routine was applied (Pouchou and Pichoir, 1991). Table 1 gives mean
Mössbauer spectroscopy (MS) was used to determine the Fe$^{3+}$/ΣFe ratio of the sample, using a conventional spectrometer system operated in constant acceleration mode (Swedish Museum of Natural History, Stockholm, Sweden). The absorber was prepared from 40 mg of ground sample mixed with an acrylic resin which was pressed to a 12-mm diameter disc under mild heating (<150°C). Data were collected over 1024 channels in the velocity range −4.2 to +4.2 mm/s using a $^{57}$Co rhodium matrix standard source of 50 mCi nominal activity and were calibrated and folded against the spectrum of an α-Fe foil. The spectrum (Fig. 2) was fit using the software MossA (Prescher et al., 2012) with three doublets assigned to Fe$^{2+}$ and one doublet assigned to Fe$^{3+}$, resulting in an Fe$^{3+}$/ΣFe ratio of 0.40, assuming similar recoil-free fractions for Fe$^{2+}$ and Fe$^{3+}$ (Table 2).

Single-crystal infrared spectroscopy

Polarised Fourier-transform infrared (FTIR) absorption spectra were measured on a 39 μm thick doubly polished single-crystal section oriented parallel to the c-axis. A Bruker Vertex 70 spectrometer attached to a Hyperion 2000 microscope was used to collect spectra in the range 2000–13000 cm$^{-1}$ at a resolution of 4 cm$^{-1}$ (Swedish Museum of Natural History, Stockholm, Sweden). Spectra recorded in polarised mode parallel to the crystallographic c-axis show a very intense band at $\sim$3570 cm$^{-1}$, which is off-scale due to excessive absorption, and three less-intense bands at 3666, 3728 and 3764 cm$^{-1}$ (Fig. 3). A shoulder occurs around 3623 cm$^{-1}$. Spectra obtained perpendicular to the c-axis show considerably weaker bands at 3577 and 3623 cm$^{-1}$, which may be the bands responsible for the very strong absorption in the opposite polarisation direction. Bands above about 3600–3650 cm$^{-1}$ are usually due to (OH) at the O(1) site (≡ W) (e.g. Gonzalez-Carreño et al., 1988; Bosi et al., 2015a). Based on the empirical crystal-chemical formula (see below) and the studies of Watenphul et al. (2016) and Bosi et al. (2018), the main FTIR bands at $\sim$3577 cm$^{-1}$ are probably

| Wt.%       | Mean (15 spots)   | Range   | S.D. | apfu |
|------------|-------------------|---------|------|------|
| SiO$_2$    | 35.45             | 34.69–36.69 | 0.42 | 5.895 |
| TiO$_2$    | 1.40              | 1.03–1.84  | 0.23 | 0.176 |
| B$_2$O$_3$ | 10.45             |          |      | 3.000 |
| Al$_2$O$_3$| 27.30             | 26.06–27.98 | 0.51 | 5.350 |
| V$_2$O$_5$ | 0.12              | 0.07–0.17  | 0.03 | 0.015 |
| FeO$_{tot}$| 5.68              | 4.11–6.36  | 0.67 | —     |
| MgO        | 11.19             | 10.55–12.13 | 0.51 | 2.774 |
| CaO        | 3.43              | 2.96–3.89  | 0.27 | 0.610 |
| Na$_2$O    | 1.10              | 0.82–1.32  | 0.14 | 0.354 |
| F          | 0.11              | 0.00–0.17  | 0.06 | 0.055 |
| H$_2$O$_a$ | 3.30              |          |      | 3.547 |
| O=F        | -0.04             |          |      | —     |
| Fe$_2$O$_b$| 2.52              |          | 0.316|  |
| FeO$_b$    | 3.41              |          | 0.474|  |
| Total      | 99.63             |          |      | —     |

Figure 2. Mössbauer spectrum of uvite. Fitted absorption doublets assigned to Fe$^{2+}$ and Fe$^{3+}$ are indicated in blue and red, respectively. Diamonds denote the measured spectrum, and the black curve represents summed fitted spectra.

Table 1. Electron microprobe data (WDS mode) and atoms per formula unit (apfu) normalised to 31 anions for uvite.  

aCalculated by stoichiometry, (Y+Z+T) = 15.00 apfu. 
bDetermined by Mössbauer spectroscopy 
S.D. – standard deviation
caused by the atomic arrangements $2[(\text{Fe,Mg})\text{AlAl}]^\cdots\text{O}(3)(\text{OH})_3$, whereas we prefer to ascribe the band at $\sim 3623$ to the arrangements $3[(\text{Fe,Mg})\text{AlAl}]^\cdots\text{O}(3)(\text{OH})_3$ rather than to $Y[(\text{Fe,Mg})\text{AlAl}]^\cdots\text{O}(1)(\text{OH})^\cdots X(\Box)$ because the $X(\Box)$ content is too low. The latter arrangement is more likely to be related to the band at $\sim 3666$ cm$^{-1}$ in the atomic arrangement $Y(\text{MgMgAl})^\cdots\text{O}(1)(\text{OH})^\cdots X(\Box)$. In this regard, note that the bands between $\sim 3650$–$3700$ cm$^{-1}$ are associated with $X(\Box)$, whereas those above $3700$ cm$^{-1}$ are associated with $X(\text{Na, Ca})$ (e.g. Gonzalez-Carreño et al., 1988; Berryman et al., 2016; Watenphul et al., 2016). Consequently, bands at $\sim 3728$ and $\sim 3764$ cm$^{-1}$ may be due to the arrangements $Y(\text{FeFeAl})^\cdots\text{O}(1)(\text{OH})^\cdots X(\text{Na})$ and $Y(\text{MgMgMg})^\cdots\text{O}(1)(\text{OH})^\cdots X(\text{Na, Ca})$, respectively.

### Table 2. Mössbauer parameters for uvite obtained at room-temperature.*

| $\delta$ (mm/s) | $\Delta E_Q$ (mm/s) | FWHM (mm/s) | $A$(%) | Assignment       |
|----------------|--------------------|-------------|--------|------------------|
| 1.08           | 2.33               | 0.28        | 21.5   | $[^{6}\text{Fe}^2+]$      |
| 1.10           | 2.56               | 0.21        | 11.7   | $[^{6}\text{Fe}^2+]$      |
| 0.97           | 1.84               | 0.64        | 26.6   | $[^{6}\text{Fe}^2+]$      |
| 0.43           | 0.81               | 0.59        | 40.2   | $[^{5}\text{Fe}^3+]$      |

* $\delta$ = centroid shift, $\Delta E_Q$ = quadrupole splitting, FWHM = full width at half-maximum, $A$ = relative area.

Optical absorption spectroscopy (OAS)

Polarised optical absorption spectra of uvite (Fig. 4) were acquired at the Natural History Museum of Stockholm, Sweden. Data were collected at room temperature on the same polished crystal that was used for FTIR measurements. An AVASPEC-ULS2048X16 spectrometer, connected via a 400 µm UV fibre cable to a Zeiss Axioshot UV-microscope, was used. A 75 W Xenon arc lamp was used as a light source and Zeiss Ultrafluor 10x lenses served as objective and condenser. A UV-quality Glan-Thompson prism, with a working range from 40000 to 3704 cm$^{-1}$, was used as the polariser.

The recorded spectra show broad and strongly polarised (O > E) absorption bands at 22000, 14250 and 8790 cm$^{-1}$ (Fig. 4). In agreement with previous optical studies of tourmaline (e.g. Mattson and Rossman, 1987), the bands at 14250 and 8790 cm$^{-1}$ are assigned to Fe$^{3+}$-enhanced spin-allowed d–d transitions in [6]-coordinated Fe$^{2+}$. The broad, intense, and strongly E||O-polarised band at 22000 cm$^{-1}$ is due to Fe$^{2+}$–Ti$^{4+}$ intervalence charge transfer processes (e.g. Smith, 1978; Taran et al., 1993).

Single-crystal structure refinement

A representative crystal of uvite from Facciatoia was selected for XRD measurements on a Bruker APEX-II single-crystal diffractometer, equipped with a Photon II CCD area detector and a graphite-crystal monochromator, using MoKα radiation from a fine-focus sealed X-ray tube (Dipartimento di Scienze della Terra, University of Pisa). The sample-to-detector distance was 5 cm. A total of 1675 exposures (step = 0.2°, time/step = 20 s) covering a full reciprocal sphere with a redundancy of $\sim 15$ was collected using $\varnothing$ and $\varnothing$ scan modes. Final unit-cell parameters were refined using the Bruker AXS SAINT’ program on reflections.

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Fig. 3. Polarised FTIR spectra for uvite. Note the presence of bands above 3650 cm$^{-1}$. The main band is truncated at $\sim 2$ absorbance units in the E||c direction due to excessive absorption. Sample thickness 39 µm.
with I > 10σ1 in the range 5° < 2θ < 72°. The intensity data were processed and corrected for Lorentzian polarisation and background effects using the APEX3 software program of Bruker AXS. The data were corrected for absorption using a multi-scan method (SADABS). The absorption correction led to an improvement in Rint (%) for 1 (%) all data 1.75 < R1 < 2 (%) 4.14

Table 3. Single-crystal X-ray diffraction data details for uvote.*

| Crystal data | 0.08 × 0.17 × 0.30 | R3m | 15.9519(10) |
| Space-group type | 7.2222(5) | c | 1591.6(2) |
| V (Å³) | 3 |

Data collection

| Data collection | MoKα λ = 0.71073 Å |
| Collection temperature (K) | 293 |
| Radiation | 5–72 |
| Range for data collection, 2θ (°) | -25 ≤ h ≤ 25; -19 ≤ k ≤ 25; -11 ≤ l ≤ 11 |
| Reciprocal space range hkl | 0.22726(15) 0.0152(3) |

| Data | 12.296 |
| Set of read reflections | 1666, 4.37 |
| Unique reflections, Rusp (%) | 1664 |
| Unique reflections with I > 2σ(I) | 15 |
| Redundancy | Multiscan (SADABS) |

Refinement

| Refinement method | Full-matrix least-squares on F² |
| Structural refinement program | SHELLX-2013 |
| Restraints, refined parameters | 2, 94 |
| Flack parameter | 0.06(3) |
| wR2 (%) | 4.14 |
| R1 (%) | 1.75 |
| R1 (%) for I > 2σI | 1.74 |
| Goof | 1.122 |
| Largest diff. hole and peak (e/Å³) | -0.66 and 0.96 |

*Notes: Rusp = merging residual value; R1 = discrepancy index, calculated from F-data; wR2 = weighted discrepancy index, calculated from F²-data; Refined as an inversion twin.

Bosi et al. (2017a). Variable parameters were as follows: scale factor, extinction coefficient, atom coordinates, site-scattering values (for X, Y and Z sites) and atomic-displacement factors. Attempts to refine the extinction coefficient yielded values within its standard uncertainty, thus it was not refined. Neutral atom scattering factors were used. In detail, the X site was first modelled using Ca versus Na, but this yielded a strong correlation (r = 0.82) between \( \delta U^{11} \) and the X site-scattering value; thus, to avoid this correlation, the X site was modelled by setting the Na content to 0.354 atoms per formula unit (apfu, see below) and allowing the remainder of the site to refine as Ca. The occupancy of the Y site was obtained considering the presence of Mg versus Fe, and the Z site with Al versus Fe. The T, B and anion sites were modelled, respectively, with Si, B and O scattering factors and with a fixed occupancy of 1, because refinement with unconstrained occupancies showed no significant deviations from this value. The position of the H(1) and H(3) atoms bonded to oxygen at the O(1) and O(3) sites, respectively, in the structure was taken from the difference-Fourier map and incorporated into the refinement model. In accord with Gatta et al. (2014), the O(1)–H(1) and O(3)–H(3) bond lengths were restrained (by DFIX command) to be 0.96 Å and 0.97 Å (respectively) with their isotropic-displacement parameters constrained to be equal to 1.2 times that obtained for the O(1) and O(3) sites. A final refinement was then done by modelling the site occupancy of the O(1) site with O and F fixed at the value obtained from the empirical formula (see below). Similar chemical constraints were applied to refine the H(1) and H(3) sites. There were no correlations greater than 0.7 between the parameters at the end of the refinement. Table 3 lists crystal data, data-collection information, and refinement details; Table 4 gives the fractional atom coordinates, equivalent isotropic-displacement parameters and Table 5 shows selected bond lengths. The crystallographic information file has been deposited with the Principal Editor of Mineralogical Magazine and is available as Supplementary material (see below).

Powder X-ray diffraction

A powder X-ray diffraction pattern for uvote was collected at the Natural History Museum of Stockholm (Sweden) using a Panalytical X'pert powder diffractometer equipped with an

Table 4. Fractional atom coordinates, isotropic (†) or equivalent-isotropic displacement parameters (in Å²) and site occupancies for uvote.

| x/a | y/b | z/c | Ueq/iso | Site occupancy |
|-----|-----|-----|---------|---------------|
| X   | 0   | 0   | 0.22726(15) | 0.0152(3) Ca0.5859(6)Na0.354 |
| Y   | 0.12374(6) | 0.06188(2) | 0.63660(8) | 0.00796(16) Mg0.8013(10)Fe0.199(10) |
| Z   | 0.29823(3) | 0.26179(3) | 0.61226(7) | 0.006264(11) Al0.9999(9)O0.006 |
| V   | 0.11005(7) | 0.22011(14) | 0.4532(3) | 0.00737(3) B1.h0 |
| T   | 0.19172(2) | 0.19001(2) | 0.00552(9) | Si1.00 |
| O(1) = W 0 | 0 | 0.7756(4) | 0.0146(5) | O0.94Fe0.055 |
| H(1) | 0.000000 | 0.909(4) | 0.0177 | H0.547 |
| O(2) | 0.000000 | 0.12303(11) | 0.47931(2) | 0.0178(3) O1.00 |
| O(3) = V 0 | 0.26500(12) | 0.13252(6) | 0.5121(2) | 0.0130(3) O1.00 |
| H(3) | 0.26402(12) | 0.13212(2) | 0.3383(3) | 0.0164* H1.00 |
| O(4) | 0.09225(6) | 0.18449(11) | 0.0717(2) | 0.0129(2) O1.00 |
| O(5) | 0.18156(11) | 0.09078(6) | 0.0918(2) | 0.0110(2) O1.00 |
| O(6) | 0.19536(7) | 0.18596(7) | 0.7787(7) | 0.00934(17) O1.00 |
| O(7) | 0.28465(7) | 0.28400(7) | 0.08006(14) | 0.00971(17) O1.00 |
| O(8) | 0.20907(9) | 0.26967(8) | 0.44147(16) | 0.01068(18) O1.00 |

*Isotropic-displacement parameters (Ueq) for H(1) and H(3) constrained to have a Ueq 1.2 times the Ueq value of the O(1) and O(3) oxygen atoms, respectively.
Table 6. Powder X-ray diffraction data for uvite.*

| h  | k  | l  | I (%) | d_{max} (Å) | d_{calc} (Å) |
|----|----|----|-------|-------------|--------------|
| 1  | 0  | 1  | 16    | 6.409       | 6.407        |
| 0  | 2  | 0  | 14    | 4.611       | 4.611        |
| 2  | 1  | 49 |       | 4.237       | 4.236        |
| 2  | 2  | 51 |       | 3.994       | 3.993        |
| 0  | 1  | 57 |       | 3.497       | 3.497        |
| 0  | 3  | 11 |       | 3.389       | 3.389        |
| 1  | 4  | 14 |       | 3.019       | 3.019        |
| 1  | 2  | 88 |       | 2.973       | 2.973        |
| 0  | 1  | 100|       | 2.584       | 2.584        |
| 0  | 2  | 15 |       | 2.409       | 2.410        |
| 0  | 3  | 16 |       | 2.385       | 2.385        |
| 0  | 1  | 12 |       | 2.197       | 2.197        |
| 0  | 2  | 16 |       | 2.169       | 2.169        |
| 1  | 0  | 11 |       | 2.135       | 2.136        |
| 0  | 2  | 8  |       | 2.118       | 2.118        |
| 2  | 3  | 20 |       | 2.063       | 2.063        |
| 1  | 5  | 53 |       | 2.047       | 2.047        |

Table 7. Refined site-scattering values and optimised site-populations for uvite.

| Site | Refined site-scattering (epfu)* | Optimised site-population (epfu) | Calculated site-scattering (epfu) |
|------|---------------------------------|---------------------------------|---------------------------------|
| X    | 15.69(9)                        | 0.61 Ca + 0.35 Na + 0.04 □      | 16.10                           |
| Y    | 47.26(24)                       | 1.50 Mg + 0.47 Fe3+ + 0.71 Al + | 47.04                           |
| Z    | 79.40(24)                       | 4.54 Al + 0.18 Fe3+ + 0.02 V3++ | 79.19                           |

* Only the reflections with I ≥ 5% are listed. The six strongest reflections are given in bold.

X'celerator silicon-strip detector. The range 5–80° (2θ) was scanned with a step-size of 0.017° with the sample mounted on a background-free Si holder using sample spinning. The diffraction data (for CuKα = 1.54059 Å), corrected using Si as an internal standard, are listed in Table 6. The program UnitCell.

Table 5. Selected bond lengths (Å) for uvite.

| X–O(2) × 3 | 2.4707(16) | B–O(6) × 2 | 1.3708(14) × 2 |
| X–O(5) × 3 | 2.6923(16) | B–O(2)      | 1.381(2)       |
| X–O(4) × 3 | 2.7854(16) | <B–O–>      | 1.374          |
| <X–O>      | 2.649      | T–O(7)      | 1.5992(10)     |

Determination of the number of atoms per formula unit

In agreement with the structure-refinement results, the boron content was assumed to be stoichiometric (B3+ = 3.00 apfu). Both the site-scattering results and the bond lengths of B and T are consistent with the B site fully occupied by boron and no amount of B3+ at the T site (e.g., Bosi and Lucchesi, 2007). The iron oxidation state was determined by MS. In accordance with Pesquera et al. (2016), the Li content was assumed to be insignificant as MgO > 2 wt.% in the sample studied. The (OH) content and the formula were then calculated by charge balance with the assumption (T + Y + Z) = 15 apfu and 31 anions pfu (Table 1). The excellent agreement between the number of electrons per formula unit (epfu) derived from EMPA and SREF (241.2 and 241.1 epfu, respectively) supports the stoichiometric assumptions.

Site populations

The uvite site populations at the X, B, T, O(3) (≡ V) and O(1) (≡ W) sites follow the standard site preference suggested for tourmaline (e.g., Henry et al., 2011) and are in accord with the information from FTIR absorption spectra (Fig. 3). The site populations at the octahedrally coordinated Y and Z sites were optimised according to the procedure of Bosi et al. (2017b), and by fixing the minor elements Ti4+ at Y and V3+ at Z.

The resulting empirical crystal-chemical formula is:

X(Ca0.61Na0.39□0.04)[Si4.50Fe2+Fe3+0.47Al0.71Fe3+0.14Ti0.18]2.33O8
Z(Al4.54Fe3+0.18V3+0.02Mg1.27)2.60(\text{[Si5.90Al1.10]6.02O18})
(BO3)3(\text{OH})6(\text{OH})6F0.03O0.40S2.00

The refined site-scattering values (Hawthorne et al., 1995) and those calculated from the site populations are compared in Table 7. The agreement between the refined and calculated values is very good, and validates the distribution of cations over the X, Y and Z sites. These site populations are also supported by the close accord of the weighted bond-valence sums and weighted atom valences (or mean formal charges) calculated from the empirical crystal-chemical formula (Table 8).

For classification purposes, the optimised formula was recast in its ordered form, i.e. with trivalent cations ordered in the Z position of the tourmaline general chemical formula (Henry et al., 2011):
Table 8. Weighted bond-valences (valence units) for uvite. a

| Site | X | Y | Z | T | B | $\Sigma_{\text{cation}}$ |
|------|---|---|---|---|---|------------------------|
| O(1) | 0.44 ±3  | 0.44 ±3  | 0.44 ±3  | 0.44 ±3  | 0.44 ±3  | 1.32 |
| O(2) | 0.21 ±1  | 0.21 ±1  | 0.21 ±1  | 0.21 ±1  | 0.21 ±1  | 0.97 |
| O(3) | 0.30 ±1  | 0.30 ±1  | 0.30 ±1  | 0.30 ±1  | 0.30 ±1  | 1.12 |
| O(4) | 0.10 ±1  | 0.10 ±1  | 0.10 ±1  | 0.10 ±1  | 0.10 ±1  | 2.07 |
| O(5) | 0.12 ±2  | 0.12 ±2  | 0.12 ±2  | 0.12 ±2  | 0.12 ±2  | 2.00 |
| O(6) | 0.43 ±1  | 0.43 ±1  | 0.43 ±1  | 0.43 ±1  | 0.43 ±1  | 2.00 |
| O(7) | 0.50 ±2  | 0.50 ±2  | 0.50 ±2  | 0.50 ±2  | 0.50 ±2  | 2.00 |
| O(8) | 0.47 ±2  | 0.47 ±2  | 0.47 ±2  | 0.47 ±2  | 0.47 ±2  | 1.99 |

*Notes: Weighted bond valence according to Bosi (2014); bond valence parameters from Gagné and Hawthorne (2015).

b Mean Formal Charge (or weighted atom valence) from the empirical crystal-chemical formula.

$$X(Ca_{0.61}Na_{0.39}O_{0.55})_2(OH)_{10} \rightarrow \Sigma(Mg_{2.35}Fe^{2+}_{0.18}Fe^{3+}_{0.08})_4 \Sigma(Si_{5.90}Al_{0.10})_6 \Sigma(O_{18})_{3.00}$$

$Z(Al_{3.25}Fe^{3+}_{3.25})_4 \Sigma(Mg_{0.42})_6 \Sigma(O_{26.06})_{0.18}$

$(BO_3)_3 \Sigma(OH)_{10.55} \Sigma(O_{0.40})_{10.00}$

End-member formula and relation to other species

The composition of the sample is consistent with a hydroxy-tourmaline belonging to the calcic group (Henry et al., 2011): it is Ca-dominant at the X position of the tourmaline general formula and hydroxy-dominant at W with $(OH)^– \rightarrow O^2–$. As divalent-cations (with Mg) are the dominant Y-constituent, formula electroneutrality requires a Z-total charge = $+17$ in the end-member formula: $CaMg_3(Al_{15}Mg)(Si_{6}O_{18})$. The unique charge arrangement compatible with the Z-constituents is $Z(Al^{3+}Mg^{2+})_3$. Therefore, the uvite end-member formula is $CaMg_3(Al_{15}Mg)(Si_{6}O_{18})$. As no tourmalines are currently approved with this composition, it can be classified as a new species.

Uvite is related to fluor-uvite, ideally $CaMg_3(Al_{15}Mg)(Si_{6}O_{18})_2(OH)_3(OH)$, by the homovalent substitutions $W(OH) \leftrightarrow W^2–$ and $YMg^{2+} \leftrightarrow ZAl^{3+}$, respectively. Uvite is also related to magnesio-lucchesiite by the heterovalent substitution $ZMg^{2+} + W(OH) \rightarrow ZAl^{3+} + W^2–$. The properties of these four tourmaline are compared in Table 9.

Calcic tourmalines from the thermal aureole of the Monte Capanne intrusion at San Piero in Campo: historical background and genetic inferences

To date, eleven tourmaline species have been identified from Elba Island. The origin of these tourmalines is both pegmatitic (elbaite, fluor-elbaite, schorl, foitite, rossmanite, tsilaisite, fluor-tsilaisite and celleriite) and non-pegmatitic related to basic hornfels (Ca-rich dravite, magnesio-lucchesiite and uvite) (e.g. Dini and Pezzotta, 2021). Among them, elbaite (Vernadsky, 1914), tsilaisite (Bosi et al., 2012), fluor-tsilaisite (Bosi et al., 2015), magnesio-lucchesiite (Scribner et al., 2021), celleriite (Bosi et al., 2022) and uvite (this study) have Elba Island as type locality. Uvite is the second calcic tourmaline, after magnesio-lucchesiite, discovered in the San Piero in Campo.
In metabasite from San Piero in Campo, calcic tourmalines (uvite and magnesio-lucchesiite) occur in the southeastern sector of the area, where metaserpentinite is in contact with intrusive rocks and are characterised by small vein systems filled by black-to-brown tourmalines. Veins are up to 2–3 cm thick and up to 1 m long. Their origin may be related to the influx of B-rich fluids released by the nearby pegmatite veins or leucocratic bodies during their crystallisation. The interaction between these B-rich fluids and (Ca/Mg)-rich metaserpentinite is consistent with the genesis of (Ca/Mg)-rich tourmalines. The compositions and the nature of the country rocks therefore require both specific host lithology and fluid interaction between these B-rich fluids and (Ca/Mg)-rich metaserpentinites during their crystallisation. The substitution mechanism between uvite and magnesio-lucchesiite relatively depleted in Mg and Al order–disorder over the Y and Z sites. In conclusion, the solid-solution between uvite and magnesio-lucchesiite is documented and shows the extreme sensitivity of the tourmaline-supergroup minerals to record subtle geochemical changes in the environment of crystallisation.

Environments of uvite formation

High Ca and low F and Al contents are essential for stabilisation of uvite in contrast to other tourmaline species such as dravite, fluor-uvite and magnesio-lucchesiite. These specific conditions therefore require both specific host lithology and fluid composition.

Uvite occurrence in mafic rocks, similar to the type locality, was noted by Scribner et al. (2018) who described uvite associated with Fe-rich dravite and Mg- and Ti-rich feruvite (and magnesio-lucchesiite; Scribner et al., 2021) in metasomatically altered lamprophyre dykes. The tourmaline formed by replacement of mafic Ca-amphibole (actinolite to magnesio-hornblende) and its specific composition was constrained by the high Ca and low Al contents in the system during the metasomatic reaction.

Although tourmaline from calc-dolomite marbles is commonly described as ‘uvite’, these tourmalines typically contain high F and/or Na contents resulting in formation of fluor-uvite–magnesio-lucchesiite or dravite–oxy-dravite–magnesio-foitite solid solutions (e.g. Bačík et al., 2012; Krmiček et al., 2021; Dutrow and Henry, 2021). The occurrence of uvite with fluor-uvite in pockets of Portage-du-Fort marble, Québec, Canada, is a notable exception (Belley et al., 2014); uvite with significant WO contents...
(ca. 0.3–0.45 apfu; recalculation of original data to electronneutral formulae) forms mainly as a late retrograde mineral replacing serendibite in generations 5 and 6 in Belley et al. (2014). Its association with fluoro-uvite and fluor-dravite (generation 4) indicates that it formed from a F- and Na-depleted fluid at the final stages of retrograde tourmaline crystallisation.

In addition to specific Ca- and Mg-rich, Al-depleted environments such as hydrothermal veins in metaserpentinites (type locality) or metasomatically altered lamprophyres (Scribner et al., 2018), uvite may also form the fluoro-uvite assemblages as a result of gradual change of fluid composition or local fluctuation in F content. The different environments and conditions that favour crystallisation of uvite show that calcic tourmalines may serve as an effective petrogenetic probe for monitoring fluid composition in hydrothermal and metamorphic systems.

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