Revision 1

Oxy-schorl, $Na(Fe^{2+}{}_2Al)Al_6Si_6O_{18}(BO_3)_3(OH)_3O$, a new mineral from Zlatá Idka, Slovak Republic and Přibyslavice, Czech Republic

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ABSTRACT

Oxy-schorl (IMA 2011-011), ideally $Na(Fe^{2+}{}_2Al)Al_6Si_6O_{18}(BO_3)_3(OH)_3O$, a new mineral species of the tourmaline supergroup, is described. In Zlatá Idka, Slovak Republic (type locality), fan-shaped aggregates of greenish black acicular crystals ranging up to 2 cm in size, forming aggregates up to 3.5 cm thick were found in extensively metasomatically altered metarhyolite pyroclastics with Qtz+Ab+Ms. In Přibyslavice, Czech Republic (co-type locality), abundant brownish black subhedral, columnar crystals of oxy-schorl, up to 1 cm in size, arranged in thin layers, or irregular clusters up to 5 cm in diameter, occur in a foliated muscovite-tourmaline orthogneiss associated with Kfs+Ab+Qtz+Ms+Bt+Grt. Oxy-schorl from both localities has a Mohs hardness of 7 with no observable cleavage and parting. The measured and calculated densities are 3.17(2) and 3.208 g cm^{-3} (Zlatá Idka) and 3.19(1) and

3.198 g cm^{-3} (Přibyslavice), respectively. In plane polarized light, oxy-schorl is pleochroic – *O* = green to bluish-green, *E* = pale yellowish to nearly colorless (Zlatá Idka) and *O* = dark greyish-green, *E* = pale brown (Přibyslavice), uniaxial negative, $\omega = 1.663(2)$, $\varepsilon = 1.641(2)$ (Zlatá Idka) and $\omega = 1.662(2)$; $\varepsilon = 1.637(2)$ (Přibyslavice). Oxy-schorl is trigonal, space group $R3m$, Z=3, $a = 15.916(3)$ Å, $c = 7.107(1)$ Å, V = 1559.1(4) Å^3 (Zlatá Idka) and $a = 15.985(1)$ Å, $c = 7.154(1)$ Å, V = 1583.1(2) Å^3 (Přibyslavice). The composition (average of 5 electron microprobe analyses from Zlatá Idka and 5 from Přibyslavice) is (in wt.%): SiO_2 33.85 (34.57), TiO_2 <0.05 (0.72), Al_2O_3 39.08 (33.55), Fe_2O_3 not determined (0.61), FeO 11.59 (13.07), MnO <0.06 (0.10), MgO 0.04 (0.74), CaO 0.30 (0.09), Na_2O 1.67 (1.76), K_2O <0.02 (0.03), F 0.26 (0.56), Cl 0.01 (<0.01), B_2O_3 (calc.) 10.39 (10.11), H_2O (from the crystal-structure refinement) 2.92 (2.72), sum 99.29 (98.41) for Zlatá Idka and Přibyslavice (in parenthesis). A combination of EMPA, Mössbauer spectroscopy and crystal-structure refinement yields empirical formulae $(Na_{0.591}Ca_{0.103}\square_{0.306})_{\Sigma 1.000}(Al_{1.885}Fe^{2+}_{1.108}Mn_{0.005}Ti_{0.002})_{\Sigma 3.000}(Al_{5.428}Mg_{0.572})_{\Sigma 6.000}(Si_{5.506}Al_{0.494})_{\Sigma 6.000}O_{18}(BO_3)_3(OH)_3(O_{0.625}OH_{0.236}F_{0.136}Cl_{0.003})_{\Sigma 1.000}$ for Zlatá Idka, and $(Na_{0.586}Ca_{0.017}K_{0.006}\square_{0.391})_{\Sigma 1.000}(Fe^{2+}_{1.879}Mn_{0.015}Al_{1.013}Ti_{0.093})_{\Sigma 3.00}(Al_{5.732}Mg_{0.190}Fe^{3+}_{0.078})_{\Sigma 6.000}(Si_{5.944}Al_{0.056})_{\Sigma 6.000}O_{18}(BO_3)_3(OH)_3(O_{0.579}F_{0.307}OH_{0.115})_{\Sigma 1.000}$ for Přibyslavice. Oxy-schorl is derived from schorl end-member by the $AlOFe_{-1}(OH)_{-1}$ substitution. The studied crystals of oxy-schorl represent two distinct ordering mechanisms: disorder of R^{2+} and R^{3+} cations in octahedral sites and all O ordered in the *W* site (Zlatá Idka), and R^{2+} and R^{3+} cations ordered in the *Y* and *Z* sites and O disordered in the *V* and *W* sites (Přibyslavice).

Keywords: oxy-schorl, tourmaline-supergroup minerals, new mineral, electron microanalysis, crystal-structure refinement, Přibyslavice, Zlatá Idka

INTRODUCTION

Minerals of tourmaline-supergroup are common in many geological environments. Complexity of their structure, variability of structural sites and chemical composition are manifested in a relatively large number of mineral species (Henry et al. 2011). Oxy-schorl, ideally $Na(Fe^{2+}{}_2Al)Al_6Si_6O_{18}(BO_3)_3(OH)_3O$, is a new member of the alkali group and oxy-series of the tourmaline supergroup (sensu nomenclature of Henry et al. 2011). The coupled general substitution ${}^{Y}R^{2+} + {}^{W}(OH) \leftrightarrow {}^{Y}Al + {}^{W}O$ derived from ideal schorl $NaFe^{2+}{}_3Al_6Si_6O_{18}(BO_3)_3(OH)_3OH$ and leading to the ideal oxy-schorl was discussed already by Foit and Rosenberg (1977); Povondra (1981), Povondra et al. (1985, 1987) and Foit (1989) published several chemical analyses of tourmalines corresponding to oxy-schorl including samples from the co-type locality Přibyslavice (Povondra et al. 1987). However, the term oxy-schorl was first introduced by Hawthorne and Henry (1999). Subsequently, oxy-schorl was described from several localities worldwide (e.g., Henry and Dutrow 2001, Novák et al. 2004, Baksheev et al. 2011). Finally, oxy-schorl was defined as a potential new species of the tourmaline supergroup in the recent tourmaline nomenclature ~~(Novák et al. 2009,~~ Henry et al. 2011). Oxy-schorl is likely quite a common mineral species; however, many tourmaline compositions are close to the simplified formula $(Na_{0.5}\square_{0.5})Fe^{2+}_{2}AlAl_{6}Si_{6}O_{18}$ $(BO_{3})_{3}$ $(OH)_{3}$ $(OH_{0.5}O_{0.5})$ (see e.g., Povondra 1981, Foit 1989, Novák et al. 2004) and owing to problems with the determination of H (and other light elements), exact classification of such schorlitic tourmalines is complicated.

Oxy-schorl was approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association under the number IMA 2011–011. The holotype material from the type locality (Zlatá Idka, Slovak Republic) is preserved in the collection of the East-Slovak Museum, Košice, Slovakia (specimen number G-12760), and in the collection of Department of Mineralogy and Petrology, Comenius University, Bratislava, Slovakia (specimen number 7279). Oxy-schorl from co-type locality (Přibyslavice, Czech Republic) is deposited in the collections of the Department of Mineralogy and Petrography, Moravian Museum, Brno, Czech Republic, specimen number B10521. We provide here a description of physical, chemical and structural characteristics of oxy-schorl as a new mineral species.

OCCURRENCE AND PHYSICAL PROPERTIES

Oxy-schorl was found in fracture fillings cutting altered metarhyolite pyroclastics, in the abandoned Marianna adit, ca 2.5 km WNW from Zlatá Idka village (48°46'7"N, 20°57'50"E), Slovak Ore Mountains (Slovenské Rudohorie), near Košice, eastern Slovakia. The acid metapyroclastic rocks of Middle Ordovician age belong to the Bystrý Potok Formation of the Gelnica Group, Gemeric Superunit, Central Western Carpathians (Vozárová et al. 2010). Associated minerals of the host-rock include quartz, albite and muscovite. Oxy-schorl is probably a product of interaction between the metarhyolite pyroclastics and boron-enriched, hydrothermal fluids generated from adjacent Permian tourmaline-bearing leucogranites. Oxy-schorl from Zlatá Idka occurs in fan-shaped aggregates of greenish black acicular crystals ranging up to 2 cm in size, with aggregates up to 3.5 cm across. Tourmaline aggregates display chemical zoning in back-scattered electron (BSE) images (Fig. 1), locally with more Mg-rich (dravite to oxy-dravite) and also *X*-site vacant composition ("□-Fe-O root name" according to Henry et al., 2011) but oxy-schorl composition prevails.

The second occurrence of oxy-schorl is in a foliated muscovite-tourmaline orthogneiss at Přibyslavice (Tisá skála outcrop, ~1 km ENE from Přibyslavice, 49°50'48"N, 15°25'1"E) near Kutná Hora, Central Bohemia Region, Czech Republic. The host Lower Palaeozoic muscovite-tourmaline alkali-feldspar granite was metamorphosed during the Variscan orogeny in the amphibolite facies (Breiter *et al*., 2010). The orthogneiss is composed of K-feldspar (orthoclase perthite), albite, quartz, muscovite, biotite, garnet and apatite with accessory zircon, magnetite, pyrite and ilmenite. Oxy-schorl from Přibyslavice formed as a primary magmatic mineral of the granite, but its composition was influenced by the later metamorphic processes (e.g., Povondra et al. 1987, 1998). It forms abundant subhedral, columnar homogeneous crystals, up to 1 cm in size, arranged in thin layers, or irregular clusters up to 5 cm in diameter.

Oxy-schorl from both localities has vitreous luster and is translucent in thin edges, non-fluorescent and paramagnetic. Its Mohs hardness is 7, it is brittle and has conchoidal fracture; cleavage and parting were not observed. The streak is pale grey. The density was measured using a pycnometric method as 3.17(2) and 3.19(1) g cm^{-3}; calculated density using empirical formula and unit-cell data yields 3.208 and 3.198 g cm^{-3} for oxy-schorl from Zlatá Idka and Přibyslavice, respectively. Oxy-schorl is negative uniaxial with the following optical properties: ω = 1.663(2), ε = 1.641(2), birefrigence: 0.022 (589.9 nm) in Zlatá Idka and ω = 1.662(2); ε = 1.637(2); birefringence: 0.025 (589.9 nm) in Přibyslavice: At both localities, oxy-schorl has distinct pleochroism; *O* = green to bluish-green, *E* = pale yellowish to nearly colorless (Zlatá Idka) and *O* = dark greyish-green, *E* = pale brown (Přibyslavice).

ANALYTICAL METHODS

Chemical composition

Representative chemical analyses (5 from Zlatá Idka, 5 from Přibyslavice) were carried out on crystals used for structure refinement using a CAMECA SX100 electron microprobe (WDS mode, 15 kV, 10 and 20 nA, 5 μm beam diameter) and the following standards: almandine (Si *K*α, Fe *K*α), titanite (Ti *K*α), sanidine (Al *K*α, K *K*α), chromite (Cr *K*α), vanadinite (*V K*α), spessartine (Mn *K*α), MgO (Mg *K*α), grossular (Ca *K*α), albite (Na *K*α), topaz (F $K\alpha$) and NaCl (Cl $K\alpha$). Detection limits of the measured elements vary between 0.01 and 0.05 wt.%. Formulae of tourmalines were calculated on a basis of 15 $Y+Z+T$ cations. H_2O was calculated on the basis of electroneutral formula and structure refinement results. The presence of H_2O was confirmed by IR spectroscopy. B_2O_3 was calculated from ideal formulae since the structure refinement data indicate full occupancy of the *B*-site and absence of $^{[4]}B$ in the *T*-site. Ti and Cl were below detection limits (0.05 and 0.01 wt.%, respectively). Analytical data are given in Table 1. The content of Li in oxy-schorl from Zlatá Idka was determined by LA-ICP-MS analysis with a laser ablation system UP 213 (New Wave, USA) and quadrupole ICP-MS spectrometer Agilent 7500 CE (Agilent, Japan), at the Central European Institute of Technology, Masaryk University, Brno. It was always lower than a detection limit which corresponded to 0.04 wt. % Li_2O. Oxy-schorl from Přibyslavice yielded $Li_2O \leq 0.06$ wt. % determined by wet chemical analysis (Povondra et al. 1987).

Mössbauer spectroscopy

The ^{57}Fe Mössbauer spectrum of powdered tourmaline (ground under acetone using an agate mortar) was acquired at constant acceleration mode using a ^{57}Co in Rh source at room temperature (293 K), at the Department of Nuclear Physics, Slovak Technical University, Bratislava, Slovakia (Zlatá Idka) and Centre for Nanomaterial Research, Faculty of Science, Palacký University in Olomouc (Přibyslavice). The isomer shift was calibrated against an α-Fe foil at room temperature. Spectra were fitted by Lorentz functions using the NORMOS program (Brand 1997) on the Zlatá Idka sample and CONFIT2000 program (Žák and Jirásková 2006) on the Přibyslavice sample. The fitting results are listed in Table 2.

Infrared spectroscopy

The FTIR spectrum of tourmaline from Přibyslavice was recorded using a Nicolet Nexus 670 spectrometer equipped with DTGS detector and XT-KBr beamsplitter. The sample was prepared by mixing 1 mg of powdered sample with 300 mg of KBr (dried beforehand at 150 °C) and pressing in an evacuated die at 10 tons. A total of 32 scans in air were carried out for the sample in the wavenumber range 4000–400 cm^{-1} at a resolution of 4 cm^{-1}. The spectrum is shown in Figure 2, and a basic interpretation of the peaks (after Reddy et al. 2007) is listed in Table 3.

Thermogravimetric analysis

Thermal decomposition of oxy-schorl from Zlatá Idka and Přibyslavice was studied in an inert atmosphere (Ar) using a simultaneous thermal analyzer (STA 449 C Jupiter, Netzsch) including both thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) in the range of 30 - 1100 °C on the Department of Inorganic Chemistry, Comenius University in Bratislava (Zlatá Idka) and Department of Physics, Palacký University in Olomouc (Přibyslavice). The sample from Zlatá Idka was placed into Pt crucible with lid and dynamically heated with a heating rate of 20 Kmin^{-1}. TG correction: 020/5000 mg, DSC correction: 020/50 mV. The Přibyslavice sample was dynamically heated in open alumina crucible with a heating rate of 5 K/min.

Powder X-ray diffraction

Powder XRD measurements of oxy-schorl from Zlatá Idka were made on the BRUKER D8 Advance diffractometer (Department of Mineralogy and Petrology, Faculty of Natural Sciences, Comenius University in Bratislava, Slovakia) under the following conditions: Bragg-Brentano geometry, Cu anticathode, Ni Kβ filters, accelerating voltage: 40 kV, beam current: 40 mA. Data was obtained by the BRUKER LynxEye detector. The step size was 0.01° 2θ, the step time was 5 s per one step, and the range of measurement was 4 – 65° $2\ \theta$. Measured data was fitted and lattice parameters were refined with DIFFRAC$^{\text{plus}}$ TOPAS software (Bruker 2010) using pseudo-Voight function. Indexed diffraction data are listed in Table 4.

Powder XRD data for oxy-schorl from Přibyslavice were recorded with a PANalytical X’Pert PRO MPD diffractometer (Co*K*α radiation) in Bragg-Brentano geometry, equipped with an X´Celerator detector and programmable divergence and diffracted beam anti-scatter slits. Diffraction pattern of the sample on a zero-background Si slide was scanned with a step size of 0.017° in 2θ range 5-90°. Data were indexed and refined with Stoe WinXPow package (version 1.06), using built-in Treor (Werner et al. 1985) and least-square refinement routines (Stoe & Cie 1999). Indexed diffraction data are listed in Table 5.

Crystal structure refinement

Single-crystal X-ray studies were carried out using a 4-circle Oxford Diffraction KM-4/Xcalibur diffractometer with a Sapphire2 (large Be window) CCD detector. The CrysAlis (Oxford Diffraction Ltd) and SHELXTL (PC Version) (Sheldrick 2000) program packages were used for data reduction and structure refinement, respectively, using neutral scattering factors and anomalous dispersion corrections. The structure of oxy-schorl was refined in *R*3*m* and converged to a final *R* index of 3.32% for Zlatá Idka and 1.91% for Přibyslavice data. Crystal and refinement details of tourmaline from Zlatá Idka are listed in Table 6, structural data are summarized in Tables 7 to 9 and bond-valence table is presented in Table 10. Crystal and refinement details of tourmaline from Přibyslavice are listed in Table 11 and structural data are summarized in Tables 12 to 14; its bond-valence table is presented in Table 15.

RESULTS

The samples of oxy-schorls from Zlatá Idka and Přibyslavice display some differences in chemical composition and site allocation. A combination of EMPA, Mössbauer spectroscopy and crystal-structure refinement yields following empirical formulae: $(\mathrm{Na}_{0.591}\mathrm{Ca}_{0.103}\ {}_{0.306})_{\Sigma 1.000}(\mathrm{Al}_{1.885}\mathrm{Fe}^{2+}_{1.108}\mathrm{Mn}_{0.005}\mathrm{Ti}_{0.002})_{\Sigma 3.000}(\mathrm{Al}_{5.428}\mathrm{Mg}_{0.572})_{\Sigma 6.000}(\mathrm{Si}_{5.506}\mathrm{Al}_{0.494})_{\Sigma 6.000}\mathrm{O}_{18}(\mathrm{BO}_3)_3(\mathrm{OH})_3(\mathrm{O}_{0.625}\mathrm{OH}_{0.236}\mathrm{F}_{0.136}\mathrm{Cl}_{0.003})_{\Sigma 1.000}$ and $(\mathrm{Na}_{0.586}\mathrm{Ca}_{0.017}\mathrm{K}_{0.006}\square_{0.391})_{\Sigma 1.000}(\mathrm{Fe}^{2+}_{1.879}\mathrm{Mn}_{0.015}\mathrm{Al}_{1.013}\mathrm{Ti}_{0.093})_{\Sigma 3.00}(\mathrm{Al}_{5.732}\mathrm{Mg}_{0.190}\mathrm{Fe}^{3+}_{0.078})_{\Sigma 6.000}(\mathrm{Si}_{5.944}\mathrm{Al}_{0.056})_{\Sigma 6.000}\mathrm{O}_{18}(\mathrm{BO}_3)_3(\mathrm{OH})_3(\mathrm{O}_{0.579}\mathrm{F}_{0.307}\mathrm{OH}_{0.115})_{\Sigma 1.000}$ for oxy-schorl from Zlatá Idka and Přibyslavice, respetively. They are in good agreement with the end-member formula $\mathrm{Na}(\mathrm{Fe}^{2+}_2\mathrm{Al})\mathrm{Al}_6\mathrm{Si}_6\mathrm{O}_{18}(\mathrm{BO}_3)_3(\mathrm{OH})_3\mathrm{O}$ requiring SiO_2 35.22, Al_2O_3 34.87, FeO 14.04, Na_2O 3.03, B_2O_3 10.20, H_2O 2.64, total 100.00 wt.%. As suggested by the empirical formulae, oxy-schorl from Zlatá Idka is moderately disordered in the octahedral sites, while disorder in oxy-schorl from Přibyslavice is only negligible.

The content of OH^- was calculated from electroneutral formula based on the crystal-structure refinement and Mössbauer spectroscopy data. Ferric iron takes only 4 % of all Fe in oxy-schorl from Přibyslavice and it was not detected in the sample from Zlatá Idka. The content of H_2O was also measured using TGA; the TGA curve shows a mass change –2.96 % (Zlatá Idka) and –2.69 % (Přibyslavice) at ca. 950-1020 °C which corresponds to breakdown of the structure and release of water (bound in form of OH^-). Reduced content of ${}^{W}\mathrm{OH}$ is also supported by the low intensity of the O–H stretching peak at 3628 cm^{-1} in the infrared absorption spectrum (Fig. 2). With regard to the possible chemical inhomogeneity of the samples (Fig. 1), the calculated H_2O contents were preferred to the TGA results.

Both tourmalines slightly differ structurally as represented by lattice parameters: *a* = 15.9134(9) Å, *c* = 7.1012 Å, V = 1557.4(2) Å^3 (powder XRD) and *a* = 15.916(3) Å, *c* = 7.107(1) Å, V = 1559.1(4) Å^3 (crystal-structure refinement) for Zlatá Idka and *a* = 15.9865(8), *c* = 7.1608(3) Å, *V* = 1584.9(2) Å^3 (powder XRD) and *a* = 15.985(1) Å, *c* = 7.154(1) Å, V = 1583.1(2) Å^3 (crystal-structure refinement) for Přibyslavice. Differences in lattice parameters result from different Fe^{2+}, Fe^{3+} and Al^{3+} occupancies in *Y*, *Z* and *T* sites in both tourmalines.

Despite all differences between studied samples, they both belong to alkali group (Fig. 3a), they represent oxy species (Fig. 3b) and their contents of Fe and Mg correspond to the composition of oxy-schorl (Fig. 3c).

DISCUSSION AND CONCLUSIONS

Oxy-schorl is chemically and structurally related to schorl. The name oxy-schorl has been abundantly used for tourmalines with the composition similar to schorl but containing more than 6.5 *apfu* Al, and O in the *W* site if known (e.g. Hawthorne & Henry 1999; Henry & Dutrow 2001; Buriánek & Novák 2004, 2007; Novák et al. 2004; Ertl et al. 2010a, 2010b; Baksheev et al. 2011; Bosi 2011). Since the current classification of the tourmaline supergroup (Henry et al. 2011) uses ordered formulae for tourmaline classification, it is generally possible to recognize oxy-schorl from electron microprobe data using the approximate limits: Na > 0.5 *apfu*, Al > 6.5 *apfu*, Fe > Mg and F < 0.5 *apfu* . However, ordering of ions in the structure of different samples can be variable. In the tourmaline structure the *W* site is located on the 3-fold axis passing through the unit cell, and surrounded by three *Y* sites (Hawthorne 1996, 2002). From the crystallographic point of view there are two different possible arrangements: 1) *W* = OH or F with valence bond ca. 0.33 *vu*; 2) *W* = O - valence bond is ca. 0.67 *vu* (*vu* = valence units, Hawthorne 1996, 2002). The substitution of O for OH results in the increase of charge requirements in the neighboring *Y* sites and the substitution of Al for divalent cations, or disorder of divalent and trivalent cations among the octahedral *Y* and *Z* sites. If the *W* site is fully occupied by O, the structural arrangements with $3^{Y}R^{2+}$ or $2^{Y}R^{2+}+^{Y}R^{3+}$ cations are less favorable than the arrangements with $3^{Y}R^{3+}$ or $2^{Y}R^{3+}+^{Y}R^{2+}$ (Hawthorne 2002). Therefore, in natural samples with the mixed occupancy of the *W* site, combination of $2^{Y}R^{2+}+^{Y}R^{3+}$ and $2^{Y}R^{3+}+^{Y}R^{2+}$ arrangements is the most probable.

The crystal-structure refinement of oxy-schorl from Zlatá Idka showed that significant amount of divalent cations is allocated in the *Z* site, resulting in the content of $^{Y}Al^{3+}$ of 1.885

apfu, the possible *Y* site short-range arrangements favor dominant O^{2-} in *W* site. The observed Al-Mg disorder in tourmalines was already studied (e.g., Grice and Ercit 1993; Hawthorne et al. 1993; Bloodaxe et al. 1999; Bosi & Lucchesi 2004). Although the Fe^{2+}-Al^{3+} disorder could be allowed by local short- and long-range arrangements (Bosi 2011), Mg is more likely substituting for Al in the *Z* site due to its smaller ionic radii similar to Al^{3+}, as was observed in the oxy-schorl from Zlatá Idka. In contrast, the oxy-schorl from Přibyslavice shows only negligible disorder of Al and (Mg,Fe) in octahedral sites; the vast majority of R^{2+} ($Fe^{2+} >>$ Mg) is allocated to the *Y* site. However, the calculated bond valence values for the *O*1 and *O*3 sites suggest a disorder of O and OH among the anion sites *V* and *W* (Table 15).

The formula of end-member oxy-schorl may be expressed either as $Na(Fe^{2+}Al_2)(Fe^{2+}Al_5)Si_6O_{18}(BO_3)_3(OH)_3O$ with cations disordered in two structural sites, or with cations disordered only in one structural site such as $NaAl_3(Al_4Fe^{2+}{}_2)Si_6O_{18}(BO_3)_3(OH)_3O$ and $Na(Fe^{2+}{}_2Al)Al_6Si_6O_{18}(BO_3)_3(OH)_3O$ – the formula used in the valid nomenclature (Henry et al. 2011). It recommends allocation of trivalent cations to the *Z* site initially, followed by assignment of the remainder of R^{3+} to *Y* site. Nevertheless, this end-member formula could not be stable owing to the local charge requirements, and the first formula with cations disordered in two sites is closely approaching the composition of natural samples (Hawthorne 2002).

These two studied oxy-schorl samples confirm the two distinct ordering mechanisms in natural oxy-tourmalines: (1) disorder of divalent and trivalent cations in octahedral sites and all O ordered in the *W* site (favored by the Mg-bearing oxy-schorl from Zlatá Idka); (2) cations ordered in the *Y* and *Z* sites and O disordered in the *V* and *W* sites (in Fe-dominant oxy-schorl from Přibyslavice). The elevated content of Mg in oxy-schorl from Zlatá Idka (Fig. 3c, Table 1) very likely facilitates higher degree of disorder in *Y* and *Z* sites and higher ordering in *W* site relative to Mg-poor oxy-schorl from Přibyslavice. Since formula with ordered *V* and *W* sites is recommended for the classification purposes (Henry et al. 2011), both compositions result in the same ordered formula that meets nomenclatural requirements for oxy-schorl.

The presence of oxy-schorl does not necessary imply oxidizing geological environment. Mineral association in the Přibyslavice orthogneiss suggests more reductive conditions documented by magnetite and pyrite (e.g., Povondra et al. 1987, 1998). Thus the reasons of the formation of oxy-schorl in spite of schorl are different than high oxygen fugacity. It could take a part in oxy-tourmalines with an increased proportion of Fe^{3+} as buergerite (e.g. Donnay et al. 1966; Grice and Ercit 1993) or povondraite component (e.g. Grice et al. 1993; Bačík et al. 2008; Baksheev et al. 2011; Novák et al. 2011), respectively, in which the deprotonization is driven by ${}^{Y}\mathrm{Fe}^{2+} + {}^{W+V}\mathrm{OH}^{-} \leftrightarrow {}^{Y}\mathrm{Fe}^{3+} + {}^{W+V}\mathrm{O}^{2-}$ reaction (Pieczka and Kraczka 2004; Bačík et al. 2011). In contrast, the deprotonization was driven by ${}^{Y}\mathrm{R}^{2+} + {}^{W+V}\mathrm{OH}^{-} \leftrightarrow {}^{Y}\mathrm{Al} + {}^{W+V}\mathrm{O}^{2-}$ reaction in studied samples of oxy-schorl from both localities. Consequently, the deprotonization in studied oxy-schorls was likely the result of local charge-balance requirements owing to the excess of Al and the formation of Al-enriched oxy-schorl is the result of the specific geochemistry of the host rock.

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Figure 1. BSE image of oxy-schorl from Zlatá Idka. The zoning is given by the variation in Fe, Mg and Al content; dark grey zone corresponds to transitional oxy-schorl to "□-Fe-O root name" tourmaline composition.

Figure 2. FTIR spectrum of oxy-schorl from Přibyslavice.

Figure 3. Ternary diagrams for minerals of tourmaline group used for determination of dominant occupancy at the *X* (a), *W* (b) and *Y* site (c).

TABLE 1. CHEMICAL COMPOSITION AND FORMULA OF OXY-SCHORL FROM ZLATÁ IDKA AND PŘIBYSLAVICE

Zlatá Idka				Přibyslavice			
SiO_2 wt%	33.10	Si *apfu*	5.506	SiO_2 wt%	34.57	Si *apfu*	5.944
TiO_2	0.02	^{Z}Al	0.494	TiO_2	0.72	^{Z}Al	0.056
B_2O_3*	10.45	Sum *T*	6.000	B_2O_3*	10.11	Sum *T*	6.000
Al_2O_3	39.81			Al_2O_3	33.55		
FeO	7.97	B	3.000	Fe_2O_3	0.61	B	3.000
MgO	2.31			FeO	13.07		
MnO	0.03	^{Z}Al	5.428	MnO	0.10	^{Z}Al	5.732
CaO	0.58	^{Z}Mg	0.572	MgO	0.74	^{Z}Mg	0.190
Na_2O	1.83	Sum *Z*	6.000	CaO	0.09	Fe^{3+}	0.078
F	0.26			K_2O	0.03	Sum *Z*	6.000
Cl	0.01	Ti	0.002	Na_2O	1.76		
H_2O**	2.92	^{Y}Al	1.885	Cl	0.00	^{Y}Al	1.013
O=F	0.11	Fe^{2+}	1.108	F	0.56	Ti^{4+}	0.093
Total	99.18	Mn	0.005	H_2O**	2.72	Fe^{2+}	1.879
		Sum *Y*	3.000	-O = F,Cl	-0.24	Mn^{2+}	0.015
				Total	98.39	Sum *Y*	3.000
		Ca	0.103				
		Na	0.591			Ca	0.017
		□	0.306			Na	0.586
		Sum *X*	1.000			K	0.006
						□	0.391
		^{V}OH	3.000			Sum *X*	1.000
		^{W}OH	0.236			^{V}OH	3.000
		F	0.136				
		Cl	0.003			^{W}OH	0.115
		O	0.625			O	0.579
		Sum *W*	1.000			F	0.307

* calculated by structural refinement; ** calculated on the basis of electroneutral formula and structure refinement results

TABLE 2. HYPERFINE PARAMETERS (MÖSSBAUER SPECTROSCOPY) OF OXY-SCHORL

	Isomer shift (mm s^{-1})	Quadrupole splitting (mm s^{-1})	Assignment	Relative abundance (%)
Zlatá Idka	0.98	2.45	$^{Y1}Fe^{2+}$	43
	0.98	2.13	$^{Y2}Fe^{2+}$	13
	0.98	1.64	$^{Y3}Fe^{2+}$	44
Přibyslavice	1.09	2.47	$^{Y1}Fe^{2+}$	37
	1.08	2.15	$^{Y2}Fe^{2+}$	35
	1.04	1.58	$^{Y3}Fe^{2+}$	25
	0.37	0.32	$^{Y}Fe^{3+}$	4

TABLE 3. IR SPECTROSCOPIC DATA FOR OXY-SCHORL FROM PŘIBYSLAVICE

Peak [cm^{-1}]	Assignment
400 – 840	lattice vibrations
840 – 1200	Si_6O_{18} stretching vibrations (Fe,Mg)-OH bending vibrations
1200 – 2000	BO_3 stretching vibrations
~ 3000 – 3600	O–H stretching (at O3; overlapping peaks from variable configurations of *Y*- and *Z*-site cations around O3)
3600 – 3700	O–H stretching (at O1; overlap of peaks from variable configurations of *Y*-site cations)

Table 4. Powder X-ray diffraction data for oxy-schorl from Zlatá Idka.

The 5 strongest lines are highlighted

h	*k*	*l*	$d_{\text{obs.}}$ [Å]	*I* [%]	$d_{\text{calc.}}$ [Å]	*h*	*k*	*l*	$d_{\text{obs.}}$ [Å]	*I* [%]	$d_{\text{calc.}}$ [Å]
1	1	0	7.957	10	7.957	1	6	1	2.01524	15	2.01524
1	0	1	6.312	49	6.312	4	4	0	1.98918	12	1.98918
0	2	1	4.9452	27	4.9452	3	4	2	1.90993	23	1.90993
3	0	0	4.5938	28	4.5938	3	5	1	1.89721	11	1.89721
2	**1**	**1**	**4.2001**	**52**	**4.2001**	1	4	3	1.86002	11	1.86001
2	**2**	**0**	**3.9784**	**100**	**3.9784**	6	2	1	1.84547	12	1.84548
0	**1**	**2**	**3.4383**	**64**	**3.4383**	7	1	0	1.82539	9	1.82540
1	3	1	3.3657	25	3.3657	6	1	2	1.80857	9	1.80857
2	0	2	3.1562	18	3.1562	3	3	3	1.76601	10	1.76601
4	0	1	3.0998	20	3.0998	1	0	4	1.76075	10	1.76074
4	1	0	3.0074	25	3.0074	6	3	0	1.73629	9	1.73630
1	**2**	**2**	**2.9338**	**52**	**2.9338**	5	3	2	1.72180	10	1.72180
3	2	1	2.8883	21	2.8883	0	2	4	1.71916	10	1.71915
3	3	0	2.6522	16	2.6522	5	4	1	1.71245	9	1.71246
3	1	2	2.6014	18	2.6014	2	6	2	1.68284	10	1.68285
0	**5**	**1**	**2.5695**	**62**	**2.5695**	2	1	4	1.68038	13	1.68037
0	4	2	2.47260	15	2.47260	0	8	1	1.67412	9	1.67412
2	4	1	2.44517	15	2.44518	0	6	3	1.64840	14	1.64840
0	0	3	2.36707	22	2.36705	2	7	1	1.63825	12	1.63825
2	3	2	2.36122	23	2.36121	5	2	3	1.61413	8	1.61412
5	1	1	2.33730	21	2.33730	1	3	4	1.61010	9	1.61010
6	0	0	2.29690	13	2.29691	5	5	0	1.59134	13	1.59134
1	1	3	2.26880	12	2.26878	4	5	2	1.58016	10	1.58016
5	2	0	2.20679	12	2.20680	4	0	4	1.57812	10	1.57811
5	0	2	2.17725	17	2.17725	8	1	1	1.57293	10	1.57293
4	3	1	2.15845	16	2.15846	8	0	2	1.54989	8	1.54989
3	0	3	2.10416	16	2.10415	3	2	4	1.54796	8	1.54796
4	2	2	2.10005	17	2.10004	4	6	1	1.54306	9	1.54307
2	2	3	2.03423	27	2.03422	9	0	0	1.53127	9	1.53127
1	5	2	2.03051	31	2.03051						

TABLE 5. POWDER X-RAY DIFFRACTION DATA FOR OXY-SCHORL FROM PŘIBYSLAVICE.

THE 5 STRONGEST LINES ARE HIGHLIGHTED

h	***k***	***l***	**$d_{\text{obs.}}$ [Å]**	***I* [%]**	**$d_{\text{calc.}}$ [Å]**	***h***	***k***	***l***	**$d_{\text{obs.}}$ [Å]**	***I* [%]**	**$d_{\text{calc.}}$ [Å]**
1	**0**	**1**	**6.3637**	**75**	**6.3604**	0	2	4	1.7333	2.0	1.7332
0	2	1	4.9775	28	4.977	5	3	2	1.7312	1.5	1.7312
3	0	0	4.6157	12	4.6149	2	6	2	1.692	1.9	1.692
2	1	1	4.2254	48	4.225	6	0	3	1.6589	14.1	1.659
2	**2**	**0**	**3.9969**	**52**	**3.9966**	2	7	1	1.6461	6.7	1.6461
0	**1**	**2**	**3.4664**	**100**	**3.4664**	1	3	4	1.6227	0.6	1.6225
1	3	1	3.3839	6	3.384	5	5	0	1.5986	7.3	1.5987
2	0	2	3.1803	1	3.1802	4	0	4	1.5896	2.4	1.5901
4	0	1	3.1164	2	3.1163	8	1	1	1.5804	0.7	1.5804
4	1	0	3.0211	8	3.0212	3	2	4	1.5591	1.0	1.5595
1	2	2	**2.9549**	**79**	**2.9549**	4	6	1	1.5504	1.9	1.5504
3	2	1	2.9035	5	2.9034	9	0	0	1.5383	1.8	1.5383
3	1	2	2.6188	3	2.6186	7	2	2	1.5293	1.6	1.5293
0	5	1	**2.5826**	**65**	**2.5826**	7	3	1	1.5221	0.8	1.5221
0	4	2	2.4883	3	2.4885	8	2	0	1.5105	2.6	1.5106
2	4	1	2.4576	3	2.4575	0	5	4	1.5033	9.3	1.5034
0	0	3	2.3868	12	2.3869	2	4	4	1.4772	2.3	1.4775
2	3	2	2.3761	16	2.376	5	1	4	1.4528	10.2	1.4529
5	1	1	2.349	9	2.349	7	4	0	1.4355	1.6	1.4356
6	0	0	2.3072	1	2.3075	0	1	5	1.4247	3.1	1.4246
1	1	3	2.2869	1	2.2871	6	5	1	1.4224	3.5	1.4224
5	2	0	2.2171	1	2.2169	4	3	4	1.4072	6.6	1.4071
5	0	2	2.1903	9	2.1904	3	8	1	1.3793	0.6	1.3794
4	3	1	2.1692	7	2.1691	10	0	1	1.3593	3.8	1.3593
3	0	3	2.12	11	2.1201	9	1	2	1.345	2.0	1.345
4	2	2	2.1125	4	2.1125	6	6	0	1.3321	1.2	1.3322
2	2	3	2.0494	12	2.0493	7	0	4	1.3277	2.8	1.3273
1	5	2	2.0423	31	2.0424	0	4	5	1.3234	1.7	1.3234
1	6	1	2.0252	5	2.0251	10	1	0	1.314	3.5	1.3141
4	4	0	1.9983	2	1.9983	8	3	2	1.3087	1.0	1.3085
3	4	2	1.9207	17	1.9208	2	3	5	1.3055	1.2	1.3056
7	0	1	1.9065	2	1.9064	9	0	3	1.2931	0.5	1.293
4	1	3	1.8729	8	1.8729	0	10	2	1.2913	0.7	1.2913
6	2	1	1.8545	4	1.8544	8	4	1	1.2869	0.8	1.2869
7	1	0	1.834	1	1.8338	9	3	0	1.2799	1.3	1.2799
6	1	2	1.8186	2	1.8187	8	2	3	1.2765	1.0	1.2764
3	3	3	1.7779	3	1.7779	5	0	5	1.272	4.1	1.2721
1	0	4	1.7754	3	1.7754						

TABLE 6. CRYSTAL AND REFINEMENT DATA FOR OXY-SCHORL FROM ZLATÁ IDKA

a = 15.916(3) Å	Space group: $R3m$
c = 7.1071(12) Å	Mo $K\alpha$ radiation, λ = 0.71073 Å
V = 1559.1(4) Å^3	Cell parameters from 1225 reflections
Z = 3	
Elongated grain, brown	0.20 × 0.10 × 0.10 mm
θ = 3.2–36.1°	($-26 \leq h \leq 17$, $-17 \leq k \leq 26$, $-11 \leq l \leq 11$)
μ = 1.68 mm^{-1}	F(000) = 1468
T = 293 K	
Reflections measured:	3174
Independent reflections:	1474
Reflections > 2σ :	1111
R [$F^2 > 2\sigma(F^2)$] = 0.034	(Δ/σ)max = <0.001
$wR(F^2)$ = 0.066	extinction coef. : none
S = 0.84	92 parameters refined
$\Delta\rho_{max}$ = 0.67 e Å^{-3}	$\Delta\rho_{min}$ = −0.38 e Å^{-3}

TABLE 7. FRACTIONAL ATOMIC COORDINATES AND ISOTROPIC OR EQUIVALENT ISOTROPIC DISPLACEMENT PARAMETERS (Å^2) OF OXY-SCHORL FROM ZLATÁ IDKA

	x	y	z	Uiso*/Ueq	Occ. (<1)
Na	0.0000	0.0000	0.0825 (5)	0.0229 (12)	0.859 (14)
Y (Al)	0.12237 (7)	0.06118 (4)	0.50346 (13)	0.0119 (3)	0.799 (7)
Y (Fe)	0.12237 (7)	0.06118 (4)	0.50346 (13)	0.0119 (3)	0.201 (7)
Z (Al)	0.29700 (6)	0.36937 (6)	1.14311 (12)	0.0104 (2)	0.959 (5)
Si	0.19214 (5)	0.19002 (5)	0.86941 (10)	0.0080 (2)	0.899 (5)
O1	0.0000	0.0000	0.6394 (8)	0.0269 (12)	
O2	0.06060 (11)	0.1212 (2)	0.3556 (4)	0.0210 (7)	
O3	0.2620 (2)	0.13101 (12)	0.3745 (4)	0.0189 (7)	
O4	0.1869 (2)	0.09346 (11)	0.9640 (4)	0.0198 (6)	
O5	−0.1883 (2)	−0.09417 (11)	−0.0580 (4)	0.0192 (6)	
O6	0.19549 (14)	0.18438 (14)	0.6403 (3)	0.0150 (4)	
O7	0.28759 (14)	0.28731 (13)	0.9447 (3)	0.0142 (4)	
O8	0.20909 (14)	0.26975 (14)	1.3046 (3)	0.0145 (4)	
B	0.10971 (18)	0.2194 (4)	0.3182 (6)	0.0142 (8)	

TABLE 8. ATOMIC DISPLACEMENT PARAMETERS (Å^2) OF OXY-SCHORL FROM ZLATÁ IDKA

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na	0.0223 (15)	0.0223 (15)	0.024 (2)	0.0111 (8)	0.000	0.000
Y (Al)	0.0113 (5)	0.0098 (4)	0.0151 (5)	0.0057 (2)	−0.0019 (3)	−0.00095 (17)
Y (Fe)	0.0113 (5)	0.0098 (4)	0.0151 (5)	0.0057 (2)	−0.0019 (3)	−0.00095 (17)
Z (Al)	0.0113 (4)	0.0109 (4)	0.0098 (4)	0.0060 (3)	0.0001 (3)	−0.0004 (3)
Si	0.0081 (4)	0.0082 (4)	0.0076 (3)	0.0041 (3)	−0.0002 (3)	−0.0008 (3)
O1	0.0314 (19)	0.0314 (19)	0.018 (3)	0.0157 (9)	0.000	0.000
O2	0.0251 (13)	0.0147 (14)	0.0197 (14)	0.0073 (7)	0.0001 (6)	0.0002 (12)
O3	0.0291 (17)	0.0171 (11)	0.0144 (13)	0.0146 (8)	0.0005 (12)	0.0003 (6)
O4	0.0243 (16)	0.0168 (10)	0.0208 (14)	0.0121 (8)	−0.0001 (12)	0.0000 (6)
O5	0.0250 (16)	0.0188 (11)	0.0160 (13)	0.0125 (8)	0.0018 (11)	0.0009 (6)
O6	0.0165 (10)	0.0169 (10)	0.0111 (8)	0.0080 (8)	0.0012 (7)	0.0008 (7)
O7	0.0135 (9)	0.0138 (9)	0.0133 (8)	0.0053 (8)	0.0002 (7)	−0.0003 (7)
O8	0.0136 (9)	0.0152 (10)	0.0153 (9)	0.0075 (8)	−0.0001 (7)	0.0018 (7)
B	0.0172 (16)	0.015 (2)	0.0094 (16)	0.0077 (10)	−0.0002 (7)	−0.0004 (14)

TABLE 9. SELECTED BOND LENGTHS FOR OXY-SCHORL FROM ZLATÁ IDKA

Site	Anion	Distance	s.d.	Site	Anion	Distance	s.d.
X	O2^{i}	2.561	(4)	***Z***	O6^{vii}	1.869	(2)
	O2^{ii}	2.561	(4)		O7	1.876	(2)
	O2	2.561	(4)		O8	1.889	(2)
	O4^{iii}	2.710	(3)		O8^{viii}	1.918	(2)
	O4^{iv}	2.710	(3)		O7^{ix}	1.925	(2)
	O4^{v}	2.710	(3)		O3^{vii}	1.9890	(15)
	O5^{i}	2.781	(3)		**avg.**	**1.911**	
	O5^{ii}	2.781	(3)				
	O5	2.781	(3)	***T***	O7	1.625	(2)
	avg.	**2.684**			O5^{x}	1.6298	(12)
					O6	1.633	(2)
Y	O1	1.944	(3)		O4	1.6412	(15)
	O6^{vi}	1.965	(2)			**1.632**	
	O6	1.965	(2)				
	O2	1.981	(2)	**B**	O2	1.380	(6)
	O2^{i}	1.981	(2)		O8^{iii}	1.373	(3)
	O3	2.132	(3)		O8^{xi}	1.373	(3)
	avg.	**1.995**			**avg.**	**1.375**	

Symmetry codes: (i) −*x*+*y*, −*x*, *z*; (ii) −*y*, *x*−*y*, *z*; (iii) *x*, *y*, *z*−1; (iv) −*y*, *x*−*y*, *z*−1; (v) −*x*+*y*, −*x*, *z*−1; (vi) *x*, *x*−*y*, *z*; (vii) −*x*+*y*+1/3, −*x*+2/3, *z*+2/3; (viii) −*x*+*y*+1/3, −*x*+2/3, *z*−1/3; (ix) −*y*+2/3, *x*−*y*+1/3, *z*+1/3; (x) −*x*+*y*, −*x*, *z*+1; (xi) −*x*+*y*, *y*, *z*−1.

Table 10. Bond valence table for oxy-schorl from Zlatá Idka

	X	*Y*	*Z*	*B*	*T*	$\sum$
	$Na_{0.591}Ca_{0.103}$ $K_{0.004}\square_{0.302}$	$Al_{1.808}$ $Fe^{2+}_{1.105}$ $Ti_{0.002}$ $Mn_{0.005}$ $Mg_{0.079}$	$Al_{5.5}$ $Mg_{0.5}$	B	$Si_{5.509}$ $Al_{0.491}$	
O1*†		0.478				1.435
O2	0.098 0.098 0.098	0.450 0.450		0.946		1.973
O3*		0.299	0.405			1.109
O4	0.065 0.065 0.065				0.960	1.986
O5	0.054 0.054 0.054				0.991	2.035
O6		0.469 0.469	0.560		0.982	2.012
O7			0.550 0.482		1.003	2.035
O8			0.531 0.491	0.995 0.995		2.016
$\sum$	0.649	2.616	3.019	2.965	3.937	
IC(avg)	0.801	2.603	2.917	3.000	3.918	
Δ	0.152	-0.013	-0.102	0.035	-0.019	

IC(avg) = average ionic charge of atoms occupying the site. *Hydrogen bond donor.
† content of the O1 site is: $O_{0.536}$ $OH_{0.328}$ $F_{0.136}$.

TABLE 11. CRYSTAL AND REFINEMENT DATA FOR OXY-SCHORL FROM PŘIBYSLAVICE

$a = 15.9853(12)$ Å	Space group: $R3m$
$c = 7.1538(6)$ Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$V = 1583.1(2)$ Å^3	Cell parameters from 2936 reflections
$Z = 3$	
Elongated grain, brown	0.30 × 0.10 × 0.10 mm
$\theta = 2.9–36.1°$	$(-26 \leq h \leq 18, -25 \leq k \leq 23, -8 \leq l \leq 11)$
$\mu = 2.20$ mm^{-1}	F(000) = 1501
$T = 293$ K	
Reflections measured:	4166
Independent reflections:	1380
Reflections > 2σ :	1285
$R\,[F^2 > 2\sigma(F^2)] = 0.0191$	(Δ/σ)max = 0.001
$wR(F^2) = 0.0400$	extinction coef. = 0.00058(10)
S = 0.98	96 parameters refined
$\Delta\rho_{max} = 0.65$ e Å^{-3}	$\Delta\rho_{min} = -0.49$ e Å^{-3}

TABLE 12. FRACTIONAL ATOMIC COORDINATES AND ISOTROPIC OR EQUIVALENT ISOTROPIC DISPLACEMENT PARAMETERS (Å^2) FOR OXY-SCHORL FROM PŘIBYSLAVICE

Site		x/a	y/b	z/c	Uiso*/Ueq	Occup.
X	Na	0	0	0.9019 (5)	0.0266 (11)	0.676(10)
Y	Fe	0.87496 (3)	0.937481 (16)	0.50264 (6)	0.00869 (12)	0.621(4)
	Al	0.87496 (3)	0.937481 (16)	0.50264 (6)	0.00869 (12)	0.379(4)
Z	Al	0.70355 (3)	0.63191 (3)	−0.14783 (6)	0.00590 (13)	0.974(3)
	Fe	0.70355 (3)	0.63191 (3)	−0.14783 (6)	0.00590 (13)	0.026(3)
T	Si	0.80806 (3)	0.81008 (3)	0.12963 (6)	0.00569 (10)	
O1	O1	0	0	0.3485 (5)	0.0363 (9)	0.69**
	F	0	0	0.3485 (5)	0.0363 (9)	0.31**
O2	O2	0.93822 (6)	0.87643 (12)	0.6435 (3)	0.0151 (4)	
O3	O3	0.73144 (14)	0.86572 (7)	0.6201 (2)	0.0123 (3)	
O4	O4	0.81267 (12)	0.90634 (6)	0.0387 (2)	0.0103 (3)	
O5	O5	0.18631 (12)	0.09316 (6)	0.0618 (2)	0.0104 (3)	
O6	O6	0.80182 (8)	0.81238 (8)	0.35415 (17)	0.0089 (2)	
O7	O7	0.71481 (8)	0.71419 (8)	0.05039 (16)	0.0086 (2)	
O8	O8	0.79017 (8)	0.72936 (8)	−0.31139 (16)	0.0097 (2)	
B	B	0.88991 (10)	0.77981 (19)	0.6753 (4)	0.0076 (4)	
H3	H3	0.735 (2)	0.8677 (12)	0.732 (5)	0.21 (2)*	

* Isotropic displacement parameter (Å^2). **Fixed according to EMPA analyses.

TABLE 13. ANISOTROPIC DISPLACEMENT PARAMETERS (Å^2) FOR OXY-SCHORL FROM PŘIBYSLAVICE

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
X	0.0267 (13)	0.0267 (13)	0.0263 (18)	0.0134 (7)	0	0
Y	0.0087 (2)	0.00611 (15)	0.0121 (2)	0.00433 (10)	−0.00216 (15)	−0.00108 (7)
Z	0.0062 (2)	0.0058 (2)	0.0058 (2)	0.00309 (18)	0.00034 (15)	−0.00008 (16)
T	0.0054 (2)	0.00520 (19)	0.0064 (2)	0.00266 (15)	−0.00021 (15)	−0.00044 (14)
O1	0.0494 (15)	0.0494 (15)	0.0102 (15)	0.0247 (8)	0	0
O2	0.0207 (7)	0.0069 (7)	0.0132 (8)	0.0035 (4)	0.0004 (3)	0.0008 (6)
O3	0.0213 (9)	0.0123 (6)	0.0063 (7)	0.0107 (4)	0.0007 (6)	0.0004 (3)
O4	0.0145 (8)	0.0074 (5)	0.0114 (8)	0.0072 (4)	0.0011 (6)	0.0006 (3)
O5	0.0149 (8)	0.0082 (5)	0.0105 (7)	0.0075 (4)	0.0012 (6)	0.0006 (3)
O6	0.0090 (5)	0.0103 (5)	0.0070 (5)	0.0047 (4)	−0.0003 (4)	−0.0009 (4)
O7	0.0088 (5)	0.0068 (5)	0.0082 (5)	0.0024 (4)	−0.0009 (4)	−0.0008 (4)
O8	0.0075 (5)	0.0115 (5)	0.0111 (5)	0.0054 (5)	0.0010 (4)	0.0021 (4)
B	0.0077 (7)	0.0074 (10)	0.0074 (10)	0.0037 (5)	0.0000 (4)	0.0000 (8)

TABLE 14. SELECTED BOND LENGTHS FOR OXY-SCHORL FROM PŘIBYSLAVICE

Site	Anion	Distance	s.d.	Site	Anion	Distance	s.d.
X	O2^{i}	2.519	(3)	***Z***	O6^{xiii}	1.8615	(13)
	O2^{ii}	2.519	(3)		O7	1.8804	(12)
	O2^{iii}	2.519	(3)		O8	1.8857	(12)
	O4^{iv}	2.772	(2)		O8^{xiv}	1.9264	(12)
	O4^{v}	2.772	(2)		O7^{xv}	1.9589	(12)
	O4^{vi}	2.772	(2)		O3^{xiii}	1.9814	(9)
	O5^{vii}	2.821	(2)		**avg.**	**1.916**	
	O5^{viii}	2.821	(2)				
	O5^{ix}	2.821	(2)	***T***	O6	1.6108	(13)
	avg.	**2.704**			O7	1.6149	(11)
					O5^{xvi}	1.6253	(7)
Y	O2	1.9941	(12)		O4	1.638	(8)
	O2^{x}	1.9942	(12)			**1.622**	
	O6^{xi}	2.0387	(13)				
	O6	2.0387	(13)	***B***	O2	1.357	(3)
	O1^{xii}	2.052	(2)		O8^{viii}	1.3841	(18)
	O3	2.1572	(19)		O8^{xvii}	1.3841	(18)
	avg.	**2.046**			**avg.**	**1.375**	

Symmetry codes: (i) *x*−1, *y*−1, *z*; (ii) −*x*+*y*, −*x*+1, *z*; (iii) −*y*+1, *x*−*y*, *z*; (iv) −*x*+*y*, −*x*+1, *z*+1; (v) *x*−1, *y*−1, *z*+1; (vi) −*y*+1, *x*−*y*, *z*+1; (vii) −*y*, *x*−*y*, *z*+1; (viii) *x*, *y*, *z*+1; (ix) −*x*+*y*, −*x*, *z*+1; (x) −*x*+*y*+1, −*x*+2, *z*; (xi) *x*, *x*−*y*+1, *z*; (xii) *x*+1, *y*+1, *z*; (xiii) −*x*+*y*+2/3, −*x*+4/3, *z*−2/3; (xiv) −*x*+*y*+2/3, −*x*+4/3, *z*+1/3; (xv) −*y*+4/3, *x*−*y*+2/3, *z*−1/3; (xvi) −*x*+*y*+1, −*x*+1, *z*; (xvii) −*x*+*y*+1, *y, z*+1.

Table 15. Bond valence table for oxy-schorl from Přibyslavice

	X	*Y*	*Z*	*B*	*T*	∑
O1*		0.363				1.088
O2	0.091 0.091 0.091	0.466 0.466		1.039		2.063
O3*		0.298	0.411			1.119
O4	0.046 0.046 0.046				0.965	1.975
O5	0.040 0.040 0.040				0.997	2.033
O6		0.415 0.415	0.571		1.033	2.020
O7			0.545 0.439		1.021	2.005
O8			0.535 0.480	0.964 0.964		1.978
∑	0.531	2.423	2.980	2.966	4.015	
IC(avg)	0.632	2.400	2.968	3.000	3.991	
Δ	0.101	-0.024	-0.012	0.034	-0.025	

IC(avg) = average ionic charge of atoms occupying the site. *Hydrogen bond donor.

Figure 1

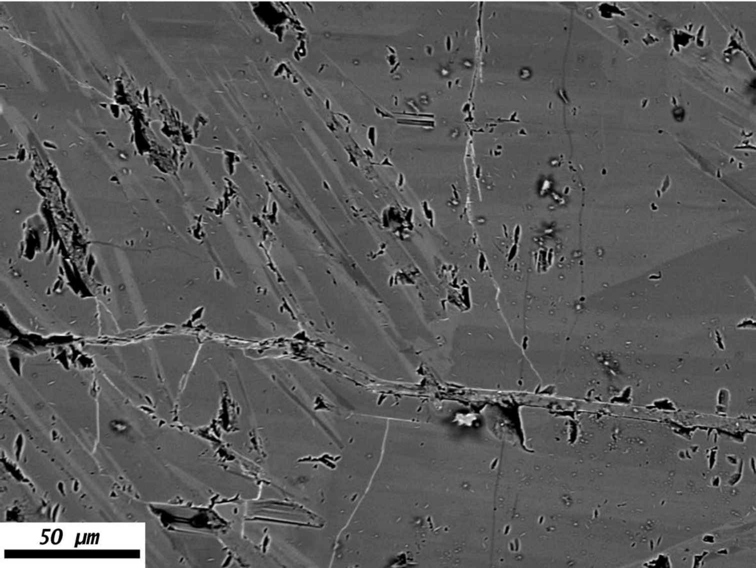
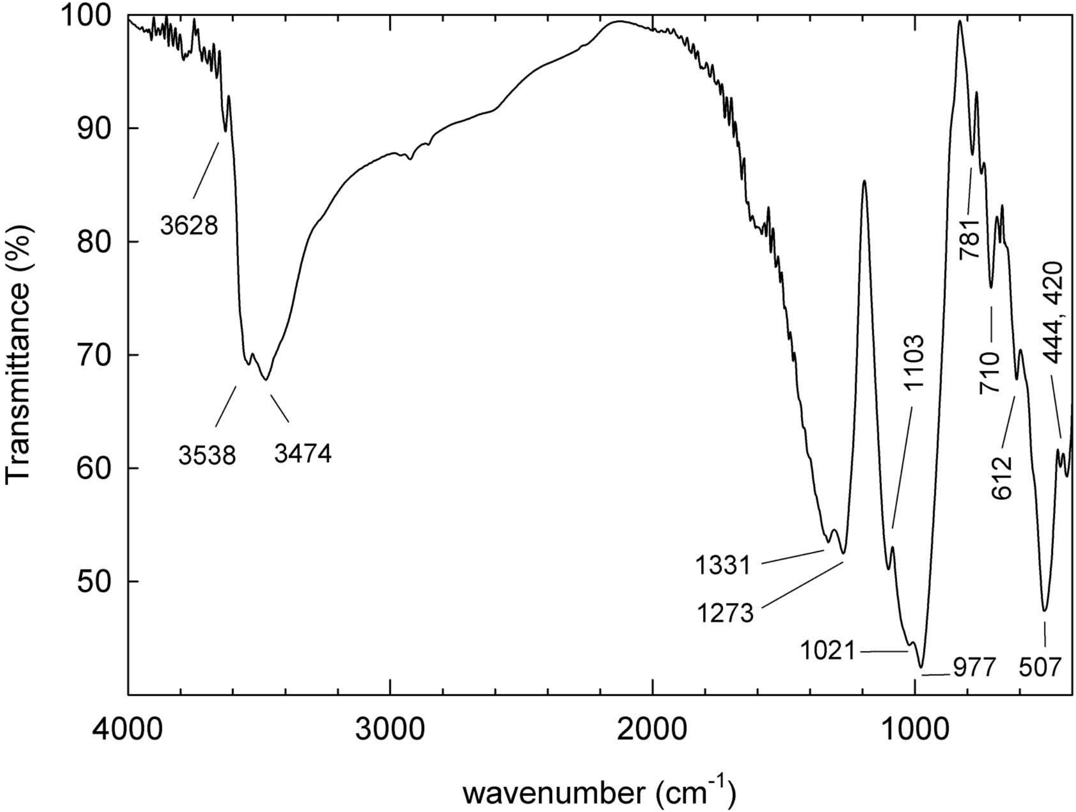


Figure 2



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60
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Transmittance (%)
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wavenumber (cm^{-1})
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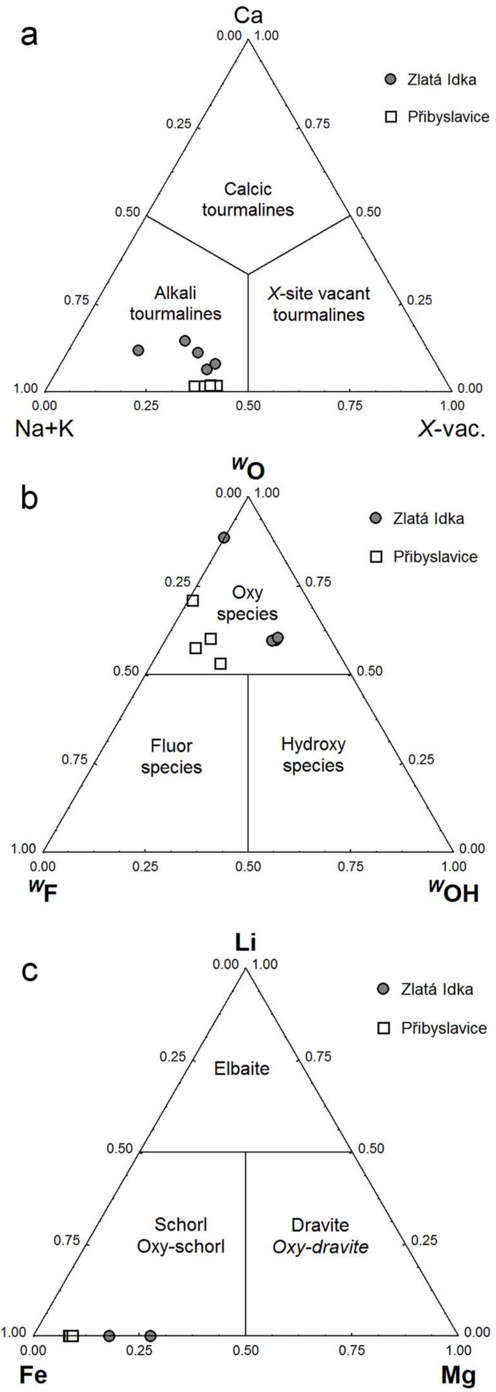
612
444, 420
507

Figure 3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Li
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Schorl
Oxy-schorl
Dravite
Oxy-dravite
Fe
Mg
Zlatá Idka
Přibyslavice