

MINERAL ASSEMBLAGES, COMPOSITIONAL VARIATION, AND CRYSTAL STRUCTURE OF FERUVITIC TOURMALINE FROM A CONTAMINATED ANATECTIC PEGMATITE AT MIROŠOV NEAR STRÁŽEK, MOLDANUBIAN ZONE, CZECH REPUBLIC

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ABSTRACT

Amphibole-bearing, simply zoned, anatectic pegmatite, up to 20 cm thick, cuts calc-silicate rocks at Mirošov, near Strážek, in the Moldanubian Zone of the Czech Republic. Common amphibole (K-rich magnesio-hornblende to ferro-hastingsite), plagioclase An_{30–42} and titanite, along with accessory feruvitic tourmaline—Ca-rich schorl to Na-rich feruvite—are indicators of Ca and Fe-contamination from the host rock. Interstitial tourmaline from the outer unit (TU1) and tourmaline from graphic intergrowths with quartz in more evolved parts of the pegmatite (TU2) have similar chemical compositions (EMPA, LA-ICP-MS) with Ca = 0.37–0.58 *apfu*, Al = 4.77–5.77 *apfu*; TU1 has higher Mg/(Mg + Fe_{tot}) = 0.52–0.41 compared to TU2 (0.39–0.15). TU1 is enriched in Ti, V, Cr, Sr, and TU2 in Li and Zn, respectively. Late microscopic veinlets of Na,Al,Mg-enriched tourmaline (TU3)—Ca-rich dravite/schorl—replace both TU1 and TU2. A combination of EMPA, single crystal XRD data, and bond-valence optimization applied to the TU2 data yielded the formula $X(Ca_{0.494}Na_{0.451}\square_{0.055})Y(Mg_{0.422}Al_{0.365}Fe^{2+}_{1.143}Fe^{3+}_{0.952}Mn_{0.029}Ti_{0.084}Zn_{0.005})Z(Al_{5.106}Fe^{3+}_{0.377}Mg_{0.518})T(Si_{5.879}Al_{0.121}O_{18})(BO_3)_3[(OH)_{2.656}O_{1.286}F_{0.058}]$, which represents disordered Na,Fe³⁺-rich feruvite (to “oxy-feruvite”). Contaminated pegmatite from Mirošov and its Ca-rich tourmalines are similar to other simple pegmatites from the Moldanubian Zone which have been contaminated by Ca,Fe-rich host rocks. The chemical compositions of Ca-rich schorl to Na-rich feruvite from various geological environments are similar, showing only minor dominance of Ca over Na (< ~0.65 *apfu* Ca), low X-site vacancy, and low Al (mostly < ~5.5 *apfu* Al), but highly variable in Mg/(Mg + Fe_{tot}). The formation of feruvite requires specific geochemical conditions with high activities of Ca and Fe, but rather low Mg, conditions typical for some contaminated granitic pegmatites.

Keywords: feruvite, schorl, EMPA, LA-ICP-MS, Mössbauer spectroscopy, powder and single crystal XRD, granitic pegmatite, contamination, Moldanubian Zone, Czech Republic

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INTRODUCTION

Feruvite is a rare member of the calcic group of tourmalines with the ideal formula $\text{CaFe}^{2+}_3(\text{Al}_5\text{Mg})(\text{BO}_3)_3(\text{Si}_6\text{O}_{18})(\text{OH})_3(\text{OH})$ (Henry *et al.* 2011). Rare occurrences of feruvite or Ca-rich schorl compositionally very close to feruvite are divided into three paragenetic groups. The first one involves Ca,Fe-rich tourmalines from tourmaline- or quartz-tourmaline veins in hydrothermally altered Ca,Al,Fe,Mg-rich host rocks including the type locality, Cuvier Island in New Zealand (Grice & Robinson 1989); feruvite from the footwall tourmalinite and quartz-tourmaline veins of the Sullivan Pb-Zn-Ag deposit in British Columbia, Canada (Jiang *et al.* 1996); Ca,Fe-rich tourmaline forming a hydrothermal breccia in a granite aureole at St. Austell, southwestern England (Manning 1991); and quartz-tourmaline hydrothermal breccia and veins within the Kerkenez granite-monzonite massif in Turkey (Demirel *et al.* 2009). The second group is represented by Ca,Fe-rich tourmalines from exocontacts of highly evolved granitic pegmatites with meta-andesite and amphibolite, such as at Red Cross Lake and Tanco, Bernic Lake, Manitoba, Canada (Selway *et al.* 1998, 2000). The third group comprises Ca,Fe-rich tourmaline from pegmatites; examples include primitive tourmaline-rich pegmatite intruding biotite-quartz augen gneiss near Cowpens, Inner Piedmont belt, South Carolina, USA (Mittwede 1984); feruvite from primitive pegmatite in hybridized diorites and granitoids near Neratovice, Teplá-Barrandien Unit, Czech Republic (Vrána 1998); and Ca,Fe-rich tourmaline from contaminated pegmatites cutting Fe-skarn at Vlastějovice nad Sázavou, in the Moldanubian Zone, Czech Republic (Novák *et al.* 2013).

Pegmatites contaminated by Fe-rich host rock can be an ideal environment for feruvite formation (*e.g.*, Novák *et al.* 2013), hence we focused on the Mirošov pegmatite. The external contamination of granitic pegmatites is a common process (Novák 2007, Černý *et al.* 2012). The degree of contamination is highly variable from almost negligible, through low (Tindle *et al.* 2002), to very strong (*e.g.*, Novák *et al.* 1999, 2012, 2013); however, the contamination of granitic pegmatites has not been systematically studied. Contamination in granitic pegmatites is indicated by the presence of Ca,Mg-rich minerals unusual for granitic pegmatites (*e.g.*, clinopyroxene, amphibole, scapolite; Novák 2007, Kuznetsova *et al.* 2010, Novák & Gadas 2010, Novák *et al.* 2012, 2013) or Ca,Mg,Fe-enriched compositions of minerals typical of granitic pegmatites, such as tourmaline (*e.g.*, Čopjaková *et al.* 2013, Novák *et al.* 1999, 2011, 2012, 2013, Tindle *et al.* 2002), garnet (Gadas *et al.* 2013), mica (Teertstra *et al.* 1995, Černý *et al.* 2003), and spodumene (Filip *et al.* 2006a).

In this paper, we describe and discuss: (1) mineral assemblages and textures of Ca,Fe-rich tourmaline from a simple anatectic pegmatite cutting lens of calc-

silicate rock; (2) crystal chemistry, crystal structure, and spectroscopy of Na-rich feruvite and Ca-rich schorl; (3) contamination of the pegmatitic melt by Ca,Fe-rich host rock; (4) relations of the Mirošov pegmatite to other simple anatectic pegmatites of the Moldanubian Zone and their tourmalines; and (5) a comparison of compositions of feruvite to Ca-rich schorl from distinct geological environments.

GEOLOGICAL SETTING

The feruvite-bearing pegmatite locality is an active quarry in strongly migmatized amphibole-biotite gneisses and amphibolites located in the southern part of the Strážek Unit at the northeastern margin of the Moldanubian Zone, ~50 km N of Brno, Czech Republic (Fig. 1). The area features a highly metamorphosed volcano-sedimentary complex composed of migmatized cordierite-biotite-sillimanite gneisses with intercalations of amphibolites, marbles, granulites, boudins of ultrabasic rocks, eclogites, and pyroxenic gneisses. The metamorphic rocks of the Strážek Unit underwent a polyphase metamorphic evolution in which high temperature-high pressure event in the upper amphibolite to granulite facies at $T_{\text{max}} \sim 850\text{--}900^\circ\text{C}$ and $P_{\text{max}} = 12\text{--}18$ kbar was overprinted during rapid decompression by an MP-HT event at $T < \sim 700^\circ\text{C}$ and $P \sim 4\text{--}6$ kbar (*e.g.*, Pertoldová *et al.* 2009, and references therein). This stage very likely produced a widespread partial melting of rocks in this region.

The main rock types found in the quarry include fine- to coarse-grained and locally strongly migmatized amphibole-biotite gneisses to amphibolites with stromatolitic to nebular textures, and layers or boudins of marbles and calc-silicate rocks, up to several m thick. Mineral assemblages of gneisses and amphibolites are simple, with dominant Ca-rich plagioclase, amphibole, Ti-rich biotite, quartz, abundant accessory garnet and titanite, and minor accessory allanite, zircon, pyrite, and apatite. These assemblages commonly contain medium- to coarse-grained segregated irregular veins and lenses of quartz + plagioclase > K-feldspar leucosome, locally with pegmatitic textures (graphic intergrowths) with amphibole, biotite, and accessory pyrite, titanite, rare diopside, and garnet as typical minerals. The calc-silicate rocks are strongly heterogeneous and locally transitional to zoned diffusive Ca-skarns formed between marbles and amphibolites (Novák 1985) with Ca-rich plagioclase, diopside, garnet, wollastonite, and accessory vesuvianite, titanite, quartz, apatite, zircon, and allanite. Primary assemblages of calc-silicate rocks are commonly replaced by amphibole, epidote, scapolite, calcite, and prehnite. Along with the rocks given above, Alpine-type veins with crystals of quartz, epidote, actinolite, chlorite, pyrite, titanite, axinite, tourmaline, and zeolites are common in the amphibolites (Černý 1955, Vávra 1994).

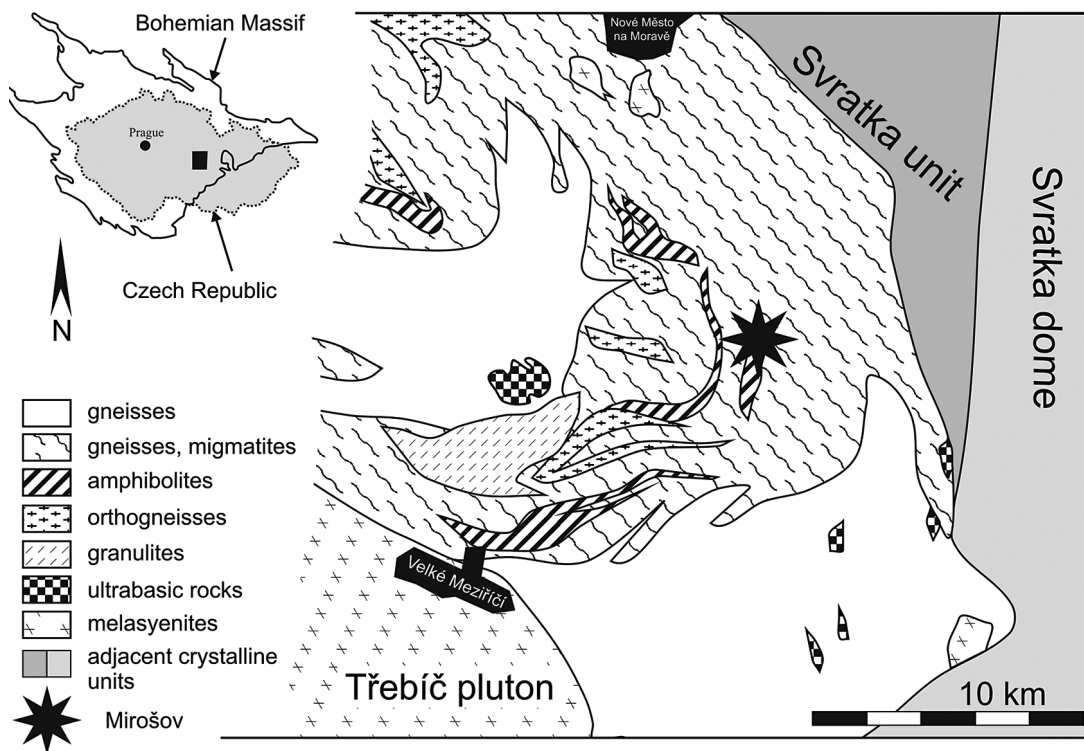


FIG. 1. Simplified geological map of the eastern part of the Strážek Unit.

METHODS

Minerals were analyzed with a Cameca SX100 electron microprobe in the Joint Laboratory of Electron Microscopy and Microanalysis, Department of Geological Sciences, Masaryk University, Brno, and Czech Geological Survey, Brno, in wavelength-dispersive mode and with accelerating voltage 15 kV, beam currents 10–20 nA, and a spot size of ~2–5 μm . The following standards and X-ray $K\alpha$ lines were used: sanidine (Si, Al, K), albite (Na), olivine (Mg), andradite (Ca, Fe), rhodonite (Mn), hornblende (Ti), chromite (Cr), topaz (F), and ZnS (Zn). The peak counting time was 10 s for major elements and 20–40 s for minor to trace elements. The background counting time was one-half of the peak counting time at the high- and low-energy background positions. The raw data were reduced using appropriate PAP matrix corrections (Pouchou & Pichoir 1985). Crystal-chemical formulae of tourmaline based solely on the EMPA data were calculated based on the general formula $XY_3Z_6T_6O_{18}(BO_3)_3V_3W$, where $X = \text{Na, Ca, K, vacancies}$; $Y = \text{Fe, Mg, Mn, Ti, Al, Zn, V}$; $Z = \text{Al, Fe, Mg}$; $T = \text{Si}$; $B = \text{B}$; $V + W = \text{OH} + \text{F} + \text{O} = 4$. Tourmaline formulae were calculated on basis of $Y + Z + T = 15 \text{ apfu}$ assuming $^7\text{Li}(\square) = 0$, $^7\text{B} = 0$, $\text{B} = 3$

apfu , and $^6\text{W}(\text{O,OH,F}) = 4 \text{ apfu}$ assuming total Fe as FeO, although the presence of Fe^{3+} was confirmed by other methods.

We carried out transmission ^{57}Fe Mössbauer spectroscopy on tourmaline sample TU2 at the Regional Centre of Advanced Technologies and Materials, Palacký University, Olomouc, Czech Republic. The spectrum of a powdered tourmaline sample (ground under acetone) was accumulated in a constant acceleration mode using a ^{57}Co in Rh source and 1024 channel detector at room temperature. The isomer shift was calibrated with regards to an $\alpha\text{-Fe}$ foil. The spectrum was folded and fitted by Lorentz functions using the computer program CONFIT2000 (Žák & Jirásková 2006).

Instrumentation for LA-ICP-MS at the Department of Chemistry, Masaryk University, Brno, consists of a UP 213 laser-ablation system (New Wave, USA) and an Agilent 7500 CE ICP-MS spectrometer (Agilent, Japan). A commercial Q-switched Nd:YAG laser ablation device operates at the fifth harmonic frequency, which corresponds to a wavelength of 213 nm. The ablation device is equipped with programmable XYZ stages to move the sample along a preset trajectory during ablation. The ablation cell was flushed with

He (carrier gas), which transported the laser-induced aerosol to the inductively coupled plasma (at 1 L/min). A gas flow of Ar to the sample was admixed to the He carrier gas flow after the laser-ablation cell. The total gas flow was 1.6 L/min. For LA-ICP-MS measurements, we used the hole drilling mode (fixed sample position during laser ablation) for 60 s for each spot. Laser ablation was performed with a laser spot diameter of 80 μm , laser fluence of 4.5 J cm⁻², and a repetition rate of 10 Hz.

The tourmaline TU2 sample was appropriate for powder XRD study. The sample was ground under isopropyl alcohol using an agate mortar and pestle. Powder X-ray diffraction (PXRD) analysis was conducted using a Bruker D8 Advance diffractometer, equipped with a Cu tube ($\lambda_{\text{K}\alpha} = 0.15418 \text{ nm}$), operated at 40 kV and 30 mA, and a 1-D position-sensitive detector at the conventional Bragg-Brentano parafocusing θ - θ reflection geometry; the step size was 0.02 $^{\circ}2\theta$, and the time per step was 188 s, over an angular range of 6–80 $^{\circ}2\theta$. Due to the small amount of pulverized material obtained, the sample was applied to a silicon monocrystal wafer. A Rietveld method-based refinement of the feruvite lattice parameters with a fundamental parameters approach (Cheary & Coelho 1992) was performed using the Bruker AXS Topas 3 software and a published feruvite structure (Grice & Ercit, 1993; obtained from AMCSD, no. 0018788) as an initial model.

The crystal structure of a TU2 tourmaline fragment was determined with a Bruker X8 APEX II diffractometer with graphite monochromated MoK α radiation at C-HORSE (the Centre for Higher Order Structure Elucidation, in the Department of Chemistry at the University of British Columbia). The crystal-to-detector distance was 37.6 mm. The data were collected at room temperature with a series of ϕ and ω scans with

0.50° oscillations and 5 s exposures. Data collection and integration was done using the Bruker SAINT software package (Bruker 2007). Data were corrected for absorption effects using the multi-scan technique (SADABS, Sheldrick 2008) and also for Lorentz and polarization effects. Experimental details and refined unit-cell dimensions of the crystals are listed in Table 1.

RESULTS

Geological setting and internal structure of pegmatite

In the eastern part of the quarry, a portion of leucosome intruded amphibolite and a small lens of more brittle calc-silicate rock forming irregularly shaped veins resembling brecciation (Fig. 2a). A pegmatitic (coarse-grained) metatect in amphibolite outside of the calc-silicate rock contains plagioclase (An_{34–50}), quartz, amphibole (K,Na,Fe,Ti-rich magnesiohornblende to tschermakite), and K-feldspar as major phases, plus minor Fe,Ti-rich phlogopite and abundant accessory titanite, along with apatite, zircon, allanite, and sulfides. The banded fine-grained calc-silicate rock is composed of heterogeneous clinopyroxene (Di_{81–47}Hd_{19–53}), garnet (Grs_{55–70}Adr_{42–22}Alm_{1–7}Prp_{0.5–1}Ti-grt_{0.5–1}), plagioclase (An_{92–94}), minor calcite and quartz with accessory titanite, apatite, zircon, and allanite. This primary mineral assemblage is strongly altered and replaced by actinolite, epidote, prehnite, and minor zeolite minerals.

An irregular pegmatite dike, up to 20 cm thick (Fig. 2b), with a more or less sharp contact with the brecciated calc-silicate rock, shows simple, irregular to symmetric zoning and the following units were recognized: (1) a narrow discontinuous reaction zone up to 5 mm thick—referred to as the contact unit—with relics of minerals from the host calc-silicate rock (Grt + Px + Amp) replaced by newly formed plagioclase, prehnite, and abundant titanite; (2) a granitic unit (Pl + Qz + Ttn) with amphibole + tourmaline (TU1) locally mutually intergrown (Fig. 3a); (3) a coarse-grained unit (Pl + Qz + Kf) with amphibole, and minor (4) graphic intergrowths of tourmaline (TU2) + quartz and K-feldspar.

Mineralogy of the pegmatite

Plagioclase forms anhedral grains in the (1) contact and (2) granitic units and subhedral crystals, up to 2 cm in length, in (3) the coarse-grained unit (Fig. 2b), with an almost identical composition in all units: (An_{30–42}Ab_{57–69}Kf_{1–4}) with traces of Sr ($\leq 0.003 \text{ apfu}$) and Fe (0.01 *apfu*). Prehnite replaced plagioclase, especially near the contact with tourmaline. The volume of K-feldspar increases inward towards the (3) coarse-grained unit and its chemical composition is quite constant (Kf_{86–91}Ab_{7–13}Cs_{0–2}) with traces of Sr. Two distinct textural types of amphibole occur in the pegmatite (Fig. 2b). Anhedral grains of amphibole I from the (2) granitic unit are slightly to strongly heterogeneous (magnesio-

TABLE 1. DATA COLLECTION AND STRUCTURE REFINEMENT INFORMATION FOR TOURMALINE TU2 FROM MIROŠOV

<i>a</i> (Å)	16.0047 (4)
<i>c</i> (Å)	7.2120 (2)
<i>V</i> (Å ³)	1599.86 (7)
<i>Z</i>	3
Radiation/ filter	MoK α /graphite
2 θ -max for data collection (°)	6.4–72.6
μ (mm ⁻¹)	2.56
Measured reflections	18675
Unique reflections	1725
Observed reflections [$> 4\sigma(F)$]	1700
<i>R</i> (int) (%)	4.1
Goodness of fit on <i>F</i> ²	1.02
<i>R</i> (%) for all data	1.5
<i>wR</i> (<i>F</i> ²) all data (%)	3.5
$\Delta\rho_{\text{max}}/\Delta\rho_{\text{min}}$	0.53/–0.49

Refinement by full-matrix least squares on *F*²

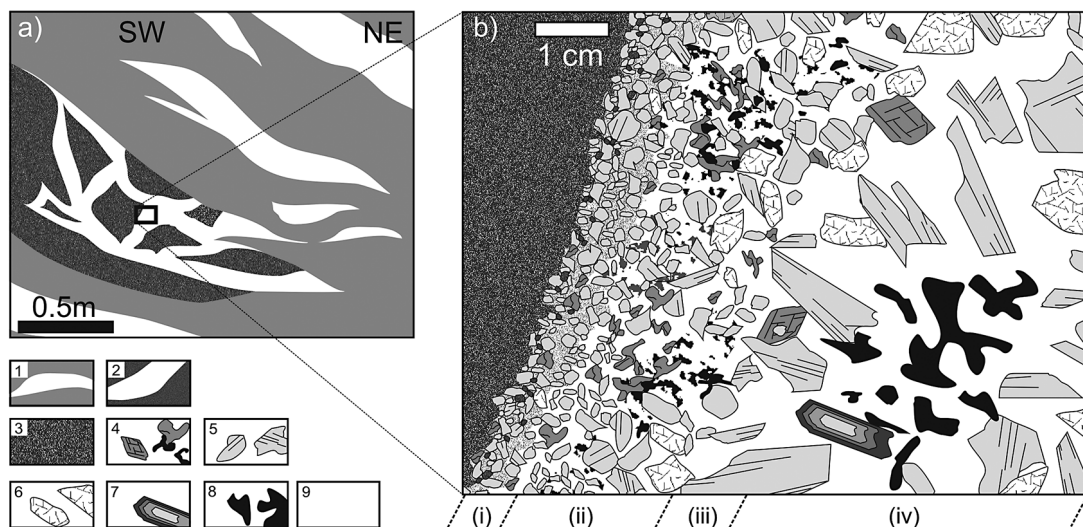


FIG. 2. Schematic diagrams showing (a) geological setting of metatects in amphibolites + pegmatite in calc-silicate rock; (b) simplified internal structure of the Mirošov pegmatite. 1 - metatect in amphibolite, 2 - pegmatite in calc silicate rock, 3 - calc silicate rock, 4 - amphibole 1 + TU1, 5 - amphibole 2, 6 - K-feldspar, 7 - allanite, 8 - TU2, 9 - quartz.

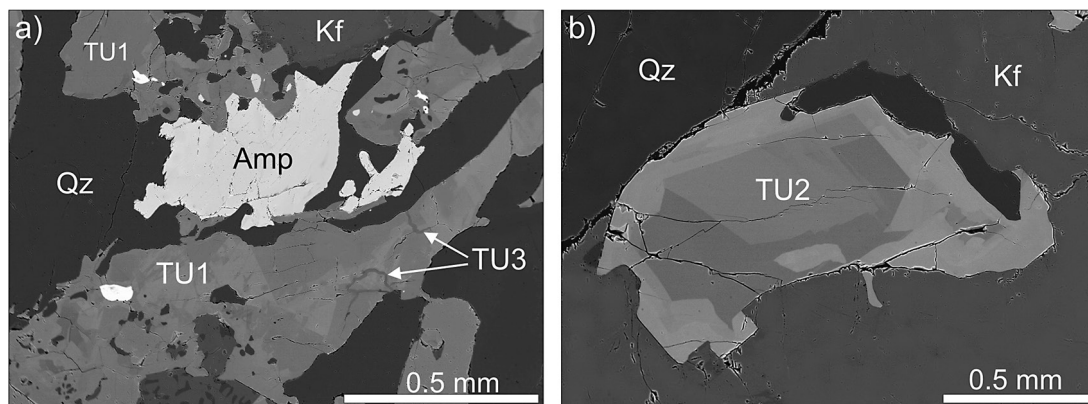


FIG. 3. BSE images of the individual textural types of tourmaline and associated minerals. (a) Anhedronal grains of TU1, locally intergrown with amphibole and veinlets of TU3 in TU1; (b) anhedronal grain of TU2 with sector zoning enclosed in K-feldspar.

hornblende to ferro-hastingsite) with $^{\text{C}}\text{Mg}/^{\text{C}}(\text{Mg}+\text{Fe}^{2+}) = 0.47\text{--}0.55$, and low to moderate contents of Na ($0.28\text{--}0.42 \text{ apfu}$) and K ($0.18\text{--}0.28 \text{ apfu}$). Euhedral crystals of amphibole II (ferro-hastingsite to potassic-ferro-hastingsite), up to 1 cm in length, from the (3) coarse grained unit with $^{\text{C}}\text{Mg}/^{\text{C}}(\text{Mg}+\text{Fe}^{2+}) = 0.30\text{--}0.47$ show elevated contents of Na ($0.41\text{--}0.52 \text{ apfu}$) and K ($0.25\text{--}0.33 \text{ apfu}$). Both amphiboles are enriched in Ti ($\leq 0.2 \text{ apfu}$) and slightly in Mn ($\leq 0.11 \text{ apfu}$), F ($\leq 0.12 \text{ apfu}$), and Cl ($\leq 0.09 \text{ apfu}$). Quartz has interstitial

character except for (4) graphic intergrowths of quartz + tourmaline. Occasionally, up to 1 cm large subhedral to euhedral crystals of REE-rich epidote occur in the central parts of the pegmatite (Fig. 2b). Titanite is the most abundant accessory mineral in all units, forming subhedral, slightly zoned, Y,REE-enriched crystals, up to 3 mm in length. Uranium-rich zircon (0.02 U apfu U and 0.02 Hf apfu), apatite, uraninite, and pyrite along with rare stibarsen, arsenopyrite, sphalerite, magnetite, and native Bi and As are present in almost all units.

Tourmaline

Tourmaline occurs in three different textural-paragenetic types. In the (2) granitic unit abundant interstitial grains of black tourmaline (TU1), up to 3 mm in length, are associated with plagioclase, quartz, K-feldspar, and amphibole (Figs. 2b, 3a). Graphic intergrowths of black tourmaline (TU2) with quartz, up to 5 cm in length, forms (4) central parts of the pegmatite dike (Fig. 2b). Microscopic veinlets and irregular discontinuous rims

of tourmaline (TU3) locally replaced both TU1 (Fig. 3a) and TU2. The TU1 and TU2 tourmalines are complexly zoned, combining sector and patchy zoning (Fig. 3a,b).

The tourmalines are compositionally variable with $Mg/(Mg + Fe_{tot}) = 0.53\text{--}0.41$ (TU1) and $0.15\text{--}0.39$ (TU2), whereas the ratios of $Ca/(Ca + Na + K)$ are comparable, $0.38\text{--}0.58$ and $0.39\text{--}0.61$, respectively (Fig. 4a). Tourmaline TU3 corresponds to Mg-rich schorl or Fe-rich dravite with $Mg/(Mg + Fe_{tot}) = 0.54\text{--}0.45$ and more variable $Ca/(Ca + Na + K) = 0.19\text{--}0.53$.

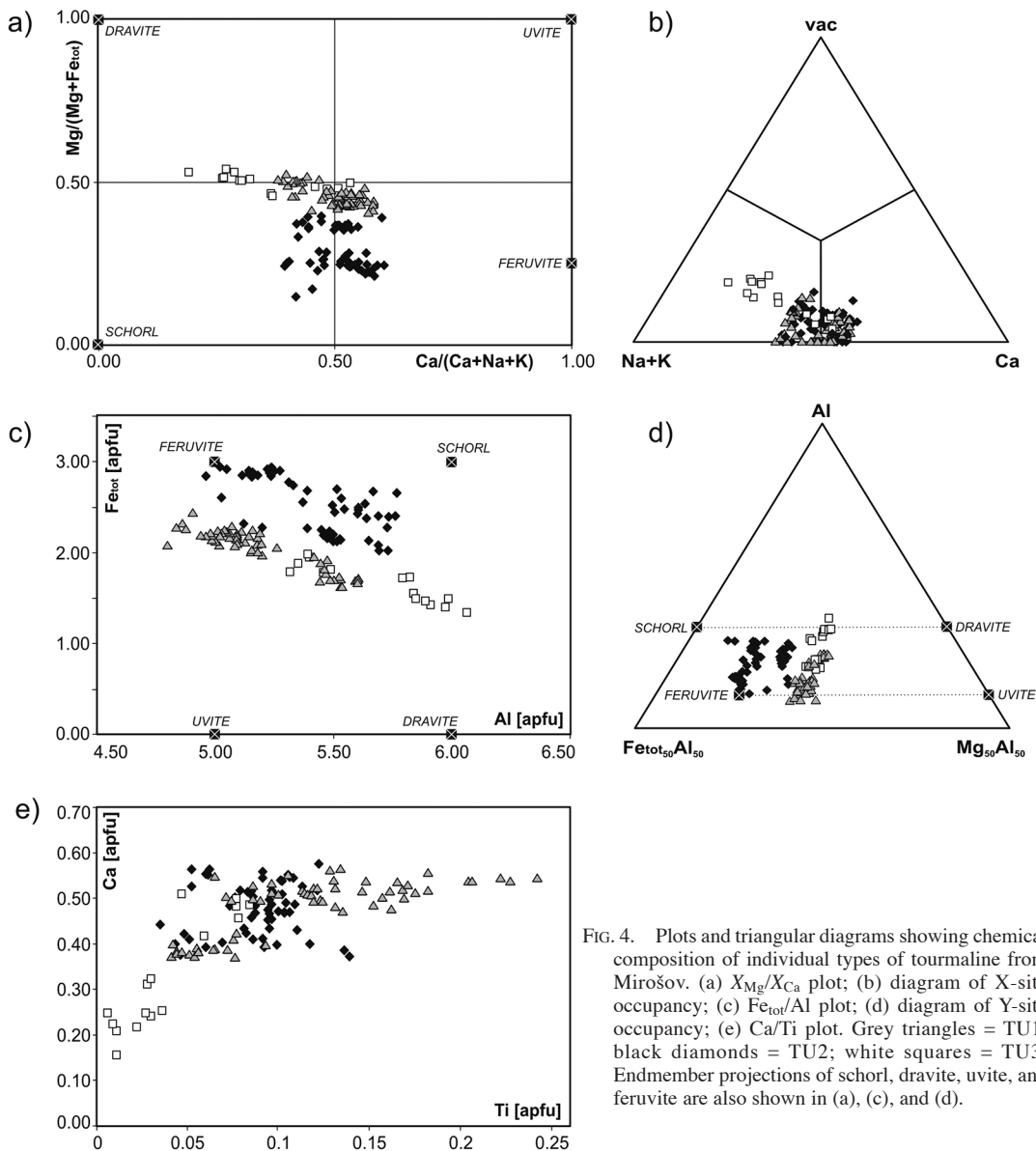


FIG. 4. Plots and triangular diagrams showing chemical composition of individual types of tourmaline from Mirošov. (a) X_{Mg}/X_{Ca} plot; (b) diagram of X-site occupancy; (c) Fe_{tot}/Al plot; (d) diagram of Y-site occupancy; (e) Ca/Ti plot. Grey triangles = TU1; black diamonds = TU2; white squares = TU3. Endmember projections of schorl, dravite, uvite, and feruvite are also shown in (a), (c), and (d).

The X-site vacancy is low to moderate in all types (Fig. 4b). Disregarding high variations of Mg and Fe in both TU1 and TU2, the studied tourmalines do not show a negative correlation for $\text{Fe}_{\text{tot}}/\text{Mg}$ in the individual types, whereas a negative correlation is apparent for $\text{Fe}_{\text{tot}}/\text{Al}$ (Fig. 4c). The Ti contents gradually decrease from TU1 (0.04–0.24 *apfu*) through TU2 (0.03–0.14 *apfu*) to TU3 (0.01–0.08 *apfu*) (Fig. 4e). The low Mn contents (~ 0.02 *apfu*) are comparable in all tourmaline types. The contents of $^{\text{W}}\text{F}$ are low and similar in TU2 (average 0.042 *apfu*) and TU3 (average 0.045 *apfu*) and slightly increased in TU1 (average 0.062 *apfu*), whereas the $^{\text{W}}\text{OH}$ contents interpolated using the formulae calculation mentioned above are apparently overestimated, as shown by increased sums of oxides. Representative compositions of tourmaline TU1, TU2, and TU3 are given in Table 2.

Only tourmaline TU2 was suitable for Mössbauer spectroscopy (Fig. 5). The Fe^{3+} content was determined as $\sim 45\%$ of total Fe (*i.e.*, including half of the intervalence charge-transfer component representing electron delocalization). The detailed spectral param-

eters and their assignment to tourmaline structural sites performed according to Andreozzi *et al.* (2008) are listed in Table 3. A detailed discussion of the role of Fe in the structure is beyond the scope of this paper. However, as reported by Andreozzi *et al.* (2008) and Bosi (2008), the assignment of the Fe doublets to Y and Z sites may be equivocal solely on the basis of Mössbauer parameters.

Because of the insufficient grain size of tourmaline TU3, only types TU1 and TU2 were analyzed for trace elements using the LA-ICP-MS equipment. Both tourmaline samples are especially enriched in V (101–502 and 53–271 ppm, respectively), Zn (135–275 and 185–495 ppm), and Sr (262–519 and 143–333 ppm). Tourmaline TU1 is slightly enriched in Cr (20–159 ppm) compared to tourmaline TU2, which is slightly enriched in Li (16–17 ppm). The Sc, Co, Ga, Sn, and Pb contents are low and comparable in both TU1 and TU2 (Table 4). Iron contents positively correlate with Zn, Ga, and Pb, whereas no correlations were observed between Fe and other trace elements. Evolutionary trends from early TU1 to more evolved TU2 are evident,

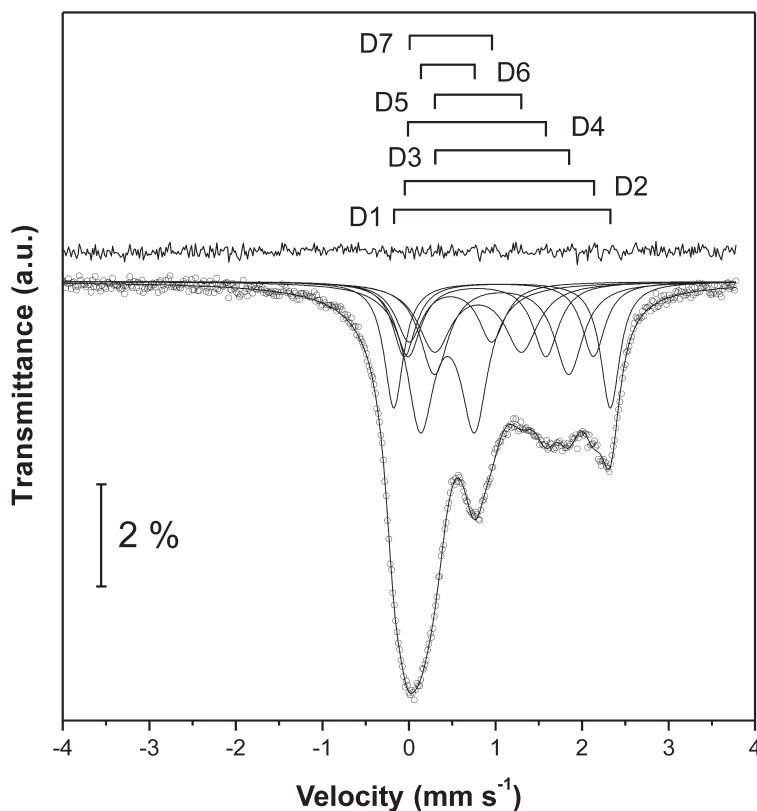


FIG. 5. Room-temperature ^{57}Fe Mössbauer spectrum of tourmaline TU2 from Mirošov.

TABLE 2. REPRESENTATIVE COMPOSITION OF TOURMALINE TU1, TU2, AND TU3 FROM MIROŠOV

	TU1					TU2					TU2 #		TU3	
SiO ₂ wt. %	34.61	34.45	34.74	34.53	34.87	35.07	34.05	34.23	34.41	34.78	33.46	35.15	35.41	36.24
TiO ₂	1.03	1.35	0.74	0.57	0.97	0.94	0.82	0.62	0.40	1.06	0.64	0.60	0.22	0.18
Al ₂ O ₃	24.95	24.79	25.29	26.02	25.62	25.73	24.84	26.97	25.47	28.01	27.00	26.93	29.41	30.75
B ₂ O ₃ *	10.10	10.14	10.19	10.22	10.25	10.19	9.93	10.04	10.03	10.11	9.89	10.25	10.36	10.55
V ₂ O ₃	0.00	0.00	0.00	0.00	0.08	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00
Fe ₂ O ₃ #											9.55			
FeO	15.08	15.63	14.71	14.33	14.08	15.90	19.51	18.58	20.04	16.62	8.22	13.67	12.29	10.17
MnO	0.07	0.12	0.10	0.09	0.15	0.00	0.14	0.09	0.16	0.41	0.20	0.11	0.09	0.00
MgO	6.54	6.50	6.99	7.06	7.17	5.72	3.60	3.06	3.34	2.98	3.59	6.41	5.94	6.64
CaO	3.05	2.77	2.78	2.69	2.70	2.82	2.89	2.33	3.02	2.10	2.62	2.64	1.73	1.23
Na ₂ O	1.17	1.45	1.26	1.37	1.50	0.99	1.31	1.43	1.28	1.74	1.32	1.35	1.63	1.83
K ₂ O	0.07	0.06	0.09	0.05	0.07	0.08	0.06	0.09	0.07	0.07	0.06	0.00	0.04	0.00
F	0.12	0.10	0.13	0.21	0.09	0.12	0.00	0.10	0.00	0.07	0.10	0.14	0.00	0.06
H ₂ O*	3.43	3.45	3.45	3.43	3.49	3.46	3.43	3.42	3.46	3.46	3.36	3.47	3.58	3.61
O=F	-0.05	-0.04	-0.05	-0.09	-0.04	-0.05	0.00	-0.04	0.00	-0.03	-0.04	-0.06	0.00	-0.03
Total	100.17	100.77	100.42	100.48	101.00	100.97	100.58	100.92	101.69	101.38	99.98	100.65	100.70	101.23
^T Si <i>apfu</i>	5.953	5.903	5.928	5.872	5.914	5.983	5.957	5.925	5.960	5.977	5.879	5.963	5.938	5.972
^T Al	0.047	0.097	0.072	0.128	0.086	0.017	0.043	0.075	0.040	0.023	0.121	0.037	0.062	0.028
B	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
Y+Z Ti	0.133	0.174	0.095	0.073	0.124	0.121	0.108	0.081	0.052	0.137	0.084	0.077	0.028	0.022
Y+Z Al	5.011	4.909	5.014	5.087	5.035	5.156	5.078	5.427	5.159	5.651	5.471	5.347	5.751	5.944
Y+Z Fe ³⁺ #											1.263			
Y+Z Fe ²⁺	2.169	2.240	2.099	2.038	1.997	2.268	2.854	2.690	2.903	2.389	1.208	1.939	1.724	1.402
Y+Z Mn	0.010	0.017	0.014	0.013	0.022	0.000	0.021	0.013	0.023	0.060	0.029	0.016	0.013	0.000
Y+Z Mg	1.677	1.660	1.778	1.790	1.813	1.455	0.939	0.790	0.862	0.764	0.940	1.621	1.485	1.631
Y+Z V	0.000	0.000	0.000	0.000	0.011	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
^X Ca	0.562	0.509	0.508	0.490	0.491	0.515	0.542	0.432	0.560	0.387	0.494	0.480	0.311	0.217
^X Na	0.390	0.482	0.417	0.452	0.493	0.327	0.444	0.480	0.430	0.580	0.451	0.444	0.530	0.585
^X K	0.015	0.009	0.020	0.011	0.015	0.017	0.013	0.020	0.010	0.015	0.000	0.000	0.009	0.000
^X vac	0.033	0.000	0.055	0.047	0.001	0.141	0.001	0.068	0.000	0.018	0.055	0.076	0.150	0.198
^V OH	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	2.720	3.000	3.000	3.000
^V O	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.220	0.000	0.000	0.000
^W F	0.065	0.054	0.070	0.113	0.048	0.065	0.000	0.055	0.000	0.038	0.058	0.075	0.000	0.031
^W OH	0.935	0.946	0.930	0.887	0.952	0.935	1.000	0.945	1.000	0.962		0.925	1.000	0.969

The compositions were established with electron-microprobe analyses. Notations: * The amounts of H₂O and B₂O₃ were calculated on the basis of stoichiometry. # calculated using single crystal XRD data (TU2).

as seen in increasing Li and Zn and decreasing V, Cr, and Sr contents.

Powder XRD data for TU2 confirm that it is tourmaline with unit cell dimensions *a* and *c* slightly higher than uvite, schorl, and dravite and close to feruvite from the type locality (Grice & Ercit 1993). The refined lattice parameters are: *a* 16.0159 (2) Å, *c* 7.2363 (1) Å, *V* = 1607.48 (5) Å³ (χ^2 = 2.58, *R*_p = 2.23, *R*_w = 3.69%). The lattice parameters of tourmaline TU2

from Mirošov are listed in Table 5, along with lattice parameters for other Fe-rich tourmalines, dravite, and uvite. The structure of TU2 obtained from single-crystal XRD was refined using the SHELXTL crystallographic software package (Sheldrick 2008) of Bruker AXS. Scattering factors for neutral atoms were employed for the cations and ionic factors for O²⁻ were used for O. The crystal structure of dravite published in Cempírek *et al.* (2013) was used as an initial model; it rapidly

converged to an R index of $\sim 2\%$ for an anisotropic displacement model. The H-atom sites were localized on residual electron density maps; their distances from donor O atoms were constrained to be approximately 0.91 Å (H3) and 0.81 Å (H1). The two most common atoms with sufficient difference in number of electrons present at the respective site were used for refinement of occupancies of X (Ca, Na), Y (Mg, Fe), and Z (Al, Fe) sites; $^T\text{Si} = 6$ was assumed since the electron density at the T site did not significantly deviate from full occupancy. The tourmaline crystal used for the collection of the X-ray intensity data was analyzed using the EMP, and the average crystal composition was employed in the final refinement and site occupancy optimization. Final atomic parameters and refined scattering values expressed as site occupancies are given in Table 6, and selected interatomic distances in Table 7.

DISCUSSION

Crystal structure of the tourmaline TU2

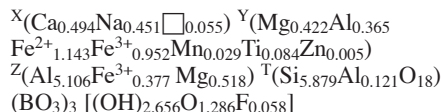
Tourmaline type TU2 was examined in detail using Mössbauer spectroscopy and single-crystal XRD structure refinement. The observed electron density at the Z site (site scattering 13.68 *epfu*) indicates the presence of Fe (minimum 0.31 *apfu* when $^Z\text{Mg} = 0$), which is otherwise mainly present at the Y site (site scattering 22.29 *epfu*); the presence of Fe at both sites is also indicated by the Mössbauer spectroscopy results. The Y and Z site occupancies were refined using least-squares bond valence (Brese & O'Keeffe 1991, Brown 2002) and electron density optimization combined with the optimization procedure of Bosi & Lucchessi (2007) as a verification tool.

The optimization of disordered Al and Mg between Y and Z sites using the Fe valences and occupancies as indicated by the Mössbauer spectroscopy results (*cf.* Table 3) led to high positive and negative residual electron densities at the Y and Z sites, respectively. The misfit between the structural data from a small crystal and those obtained from a comparatively large Mössbauer spectroscopy sample is understandable with regard to the inhomogeneous feruvite composition in the terms of Fe_{tot} (Fig. 4c) as well as the uncertainty in site assignment based on Mössbauer spectra alone (*e.g.*, Andreozzi *et al.* 2008, Bosi 2008).

The formula optimization using Al and Mg disordered between the Y and Z sites, without $\text{Fe}^{3+}/\text{Fe}_{\text{tot}}$ constraints and with both $^Z\text{Fe}^{2+}$ and $^Z\text{Fe}^{3+}$, had too many free variables and showed several local minima with $\text{Fe}^{3+} \gg \text{Fe}^{2+}$. No significant disorder of Fe^{2+} between the Y and Z sites in the studied tourmaline structure can be shown using the formula optimization. The disorder was suggested earlier on the basis of structure refinement optimization combined with Mössbauer spectroscopy (*e.g.*, Andreozzi *et al.* 2008, Bosi 2008, Filip *et al.*

2012), but has not been verified by other techniques (*cf.* Ertl *et al.* 2012, Bosi & Andreozzi 2013).

Finally, the bond-valence and electron density optimization using Al and Mg disordered between the Y and Z sites, no $\text{Fe}^{3+}/\text{Fe}_{\text{tot}}$ constraint, and with all ^ZFe as Fe^{3+} , led to the following structural formula:



Verification using the optimization procedure of Bosi & Lucchessi (2007) combined with electron density

TABLE 3. ROOM-TEMPERATURE ^{57}Fe MOSSBAUER HYPERFINE PARAMETERS FOR TOURMALINE TU2 FROM MIROŠOV (FIG. 5)

Doublet Valence of iron Parameter			Value – TU2 Assignment	
D1	Fe^{2+}	δ (mm s $^{-1}$)	1.08	Y1 site
		ΔE_Q (mm s $^{-1}$)	2.50	
		Γ (mm s $^{-1}$)	0.27	
		RA (%)	15	
D2	Fe^{2+}	δ (mm s $^{-1}$)	1.04	Y2 site
		ΔE_Q (mm s $^{-1}$)	2.19	
		Γ (mm s $^{-1}$)	0.32	
		RA (%)	11	
D3	Fe^{2+}	δ (mm s $^{-1}$)	1.07	Y3 site
		ΔE_Q (mm s $^{-1}$)	1.55	
		Γ (mm s $^{-1}$)	0.40	
		RA (%)	16	
D4	$\text{Fe}^{2.5+}$	δ (mm s $^{-1}$)	0.79	ED
		ΔE_Q (mm s $^{-1}$)	1.59	
		Γ (mm s $^{-1}$)	0.36	
		RA (%)	12	
D5	$\text{Fe}^{2.5+}$	δ (mm s $^{-1}$)	0.80	ED
		ΔE_Q (mm s $^{-1}$)	1.01	
		Γ (mm s $^{-1}$)	0.46	
		RA (%)	14	
D6	Fe^{3+}	δ (mm s $^{-1}$)	0.45	Y site
		ΔE_Q (mm s $^{-1}$)	0.62	
		Γ (mm s $^{-1}$)	0.38	
		RA (%)	23	
D7	Fe^{3+}	δ (mm s $^{-1}$)	0.48	Z site
		ΔE_Q (mm s $^{-1}$)	0.96	
		Γ (mm s $^{-1}$)	0.37	
		RA (%)	9	

Notations: δ – isomer shift (± 0.02 mm s $^{-1}$), ΔE_Q – quadrupole splitting (± 0.02 mm s $^{-1}$), Γ – peak width (± 0.02 mm s $^{-1}$), RA – relative area in the spectrum ($\pm 3\%$) and ED – electron delocalization.

TABLE 4. CONCENTRATION OF TRACE ELEMENTS (MEDIAN) FOR TOURMALINE TU1 AND TU2 FROM MIROŠOV

element	TU1			TU2			d.l.
	range	$\bar{\sigma}$	<i>M</i>	range	$\bar{\sigma}$	<i>M</i>	
Li	b.d.l.	-	-	16 – 70	16	53	16
Sc	b.d.l. – 37	12	35	b.d.l. – 23	8	14	9
V	101 – 502	118	285	53 – 271	53	70	0.3
Cr	b.d.l. – 159	43	36	b.d.l.	-	-	14
Co	14 – 27	4	19	b.d.l. – 18	7	15	13
Zn	135 – 275	44	186	185 – 495	43	345	8
Ga	40 – 98	16	62	36 – 71	11	49	11
Sr	262 – 519	69	337	143 – 333	44	228	1
Sn	6 – 19	4	10	5 – 13	2	9	1
Pb	12 – 34	6	23	16 – 36	4	21	3

Notations: d.l.: detection limits, b.d.l.: below detection limit, $\bar{\sigma}$: standard deviation, *M*: median. Concentrations are quoted in ppm.

TABLE 5. THE LATTICE PARAMETERS OF TOURMALINE TU2 FROM MIROŠOV AND OTHER Fe-RICH TOURMALINES, DRAVITE, AND UVITE

	<i>a</i> [Å]	<i>c</i> [Å]	source
tourmaline TU2 (powder XRD)	16.016	7.236	Mirošov – this work
tourmaline TU2 (single-crystal XRD)	16.0047	7.212	Mirošov – this work
feruvite	16.000	7.248	Grice & Ercit (1993)
povondraite	16.19	7.44	Henry <i>et al.</i> (2011)
schorl	15.98	7.16	Henry <i>et al.</i> (2011)
uvite	15.954	7.214	Henry <i>et al.</i> (2011)
dravite	15.96	7.21	Henry <i>et al.</i> (2011)
fluor-buergerite	15.87	7.19	Henry <i>et al.</i> (2011)

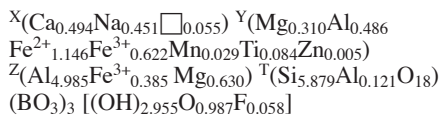
TABLE 6. FRACTIONAL ATOMIC COORDINATES AND ISOTROPIC OR EQUIVALENT ISOTROPIC DISPLACEMENT PARAMETERS ($\text{\AA}^2$) FOR TOURMALINE TU2 FROM MIROŠOV

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Ca	0.0000	0.0000	0.21562 (14)	0.0147 (3)	0.424 (12)
Na	0.0000	0.0000	0.21562 (14)	0.0147 (3)	0.576 (12)
YFe	0.121449 (18)	0.060724 (9)	0.63711 (6)	0.00735 (8)	0.735 (4)
YMg	0.121449 (18)	0.060724 (9)	0.63711 (6)	0.00735 (8)	0.265 (4)
ZAl	0.298212 (19)	0.26149 (2)	0.61103 (6)	0.00476 (8)	0.948 (2)
ZFe	0.298212 (19)	0.26149 (2)	0.61103 (6)	0.00476 (8)	0.052 (2)
Si	0.191762 (17)	0.190127 (18)	0.0000	0.00432 (6)	
B	0.11020 (5)	0.22040 (10)	0.4522 (2)	0.0060 (2)	
O1	0.0000	0.0000	0.7867 (4)	0.0186 (4)	
O2	0.06085 (4)	0.12169 (7)	0.4760 (2)	0.0106 (2)	
O3	0.26752 (9)	0.13376 (4)	0.51154 (18)	0.01124 (19)	
O4	0.09233 (4)	0.18466 (8)	0.07091 (17)	0.00881 (18)	
O5	0.18308 (8)	0.09154 (4)	0.09101 (17)	0.00908 (18)	
O6	0.19644 (5)	0.18751 (5)	-0.22206 (13)	0.00735 (12)	
O7	0.28480 (5)	0.28448 (5)	0.07979 (12)	0.00767 (13)	
O8	0.20935 (5)	0.27013 (5)	0.44104 (13)	0.00898 (13)	
H3	0.261 (3)	0.1307 (16)	0.390 (6)	0.067 (13)*	
H1	0.0000	0.0000	0.898 (11)	0.34 (13)*	

TABLE 6. (CONTINUED) ANISOTROPIC ATOMIC DISPLACEMENT PARAMETERS

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca	0.0121 (4)	0.0121 (4)	0.0201 (5)	0.00603 (18)	0.000	0.000
Na	0.0121 (4)	0.0121 (4)	0.0201 (5)	0.00603 (18)	0.000	0.000
YFe	0.00829 (11)	0.00509 (9)	0.00973 (14)	0.00415 (5)	-0.00384 (7)	-0.00192 (4)
YMg	0.00829 (11)	0.00509 (9)	0.00973 (14)	0.00415 (5)	-0.00384 (7)	-0.00192 (4)
ZAl	0.00461 (12)	0.00495 (12)	0.00453 (13)	0.00224 (9)	0.00001 (8)	0.00052 (9)
ZFe	0.00461 (12)	0.00495 (12)	0.00453 (13)	0.00224 (9)	0.00001 (8)	0.00052 (9)
Si	0.00415 (10)	0.00384 (10)	0.00483 (13)	0.00189 (7)	-0.00029 (8)	-0.00059 (8)
B	0.0056 (4)	0.0059 (5)	0.0067 (6)	0.0030 (2)	0.0002 (2)	0.0005 (4)
O1	0.0176 (6)	0.0176 (6)	0.0205 (12)	0.0088 (3)	0.000	0.000
O2	0.0113 (3)	0.0049 (4)	0.0135 (6)	0.00243 (19)	0.00079 (16)	0.0016 (3)
O3	0.0189 (5)	0.0123 (3)	0.0046 (5)	0.0095 (2)	0.0011 (4)	0.00055 (18)
O4	0.0066 (3)	0.0133 (4)	0.0088 (5)	0.0066 (2)	-0.00043 (17)	-0.0009 (3)
O5	0.0141 (4)	0.0064 (3)	0.0093 (5)	0.0070 (2)	0.0017 (4)	0.00086 (18)
O6	0.0085 (3)	0.0083 (3)	0.0050 (3)	0.0040 (2)	-0.0002 (2)	-0.0011 (2)
O7	0.0067 (3)	0.0057 (3)	0.0082 (3)	0.0013 (2)	-0.0021 (2)	-0.0013 (2)
O8	0.0040 (2)	0.0089 (3)	0.0137 (4)	0.0030 (2)	0.0010 (2)	0.0023 (2)

optimization yielded a similar formula with slightly different Al-Mg arrangement and lower $\text{Fe}^{3+}/\text{Fe}_{\text{tot}}$:



The mismatch between the two results stems from the different optimization approaches and different constants used (general bond-valence parameters *versus* ionic radii optimized for the tourmaline structure). In general, the difference is rather small with regard to the precision limits of EMP and single-crystal XRD methods. Both results fit the refined electron densities at the cation sites [$\Delta\text{X} = 0.025 \text{ e}^-$; $\Delta\text{e}(\text{Y}) = 0.040 \text{ e}^-$; $\Delta\text{e}(\text{Z}) = 0.049 \text{ e}^-$; $\Delta\text{e}(\text{T}) = -0.02 \text{ e}^-$] equally well. The first formula matches the optimal valences of all cation and anion sites slightly better than the second. The latter formula has $\text{Fe}^{3+}/\text{Fe}_{\text{tot}} = 0.41$, which is closer to the value obtained experimentally by Mössbauer spectroscopy for the heterogeneous TU2 sample ($\text{Fe}^{3+}/\text{Fe}_{\text{tot}} = 0.45$) compared to the relatively high $\text{Fe}^{3+}/\text{Fe}_{\text{tot}} = 0.54$ in the first formula. With regard to the robust nature of the bond-valence constants which are derived from stoichiometric compounds without occupational disorder (Brese & O'Keeffe 1991), we prefer the first formula optimized using the bond-valence model. At the same time, we acknowledge that the true values most likely lie between the two optimized results.

Both formulae above represent disordered Na,Fe^{3+} -rich feruvite in a solid solution with povondraite (indicated by high Na and Fe^{3+}) and oxy-schorl and/or oxy-dravite (indicated by elevated Al > 5). However, if emphasizing the role of Ca as the major element at the X site, it also may be interpreted as an oxy-tourmaline (“oxy-feruvite”) with the ideal formula

$\text{CaFe}^{2+}_3\text{Al}_6\text{Si}_6\text{O}_{18}(\text{BO}_3)_3(\text{OH})_3\text{O}$: calcic-subgroup 3 and Ca-Fe-O root name (see Henry *et al.* 2011) derived from feruvite by the substitution $^{\text{Z}}\text{R}^{3+}\text{WO} = ^{\text{Z}}\text{R}^{2+}\text{WOH}$, where R^{3+} is dominated by Al and R^{2+} by Fe^{2+} , respectively.

The observed <T–O> bond length (1.623 Å) and bond valence of the T site confirm the presence of minor $^{\text{T}}\text{Al}^{3+}$ as suggested by the EMP formula calculation. The refined elevated amounts of $^{\text{T}}\text{Al}$ are a typical feature of various R^{3+} -rich tourmalines (*e.g.*, 0.4 *apfu* $^{\text{T}}\text{Al}$ in olenite, Cempírek *et al.* 2006; 0.494 *apfu* $^{\text{T}}\text{Al}$ in oxy-schorl, Bačík *et al.* 2013).

The refined high contents of Ca are reflected in relatively short <X–O> (2.660 Å) compared to Na-dominant tourmalines; comparable low values were observed in uvite (*e.g.*, Taylor *et al.* 1995) and feruvite (Grice & Robinson 1989). Similar high Ca contents were sometimes observed in tourmaline of oxy-schorl–oxy-dravite solid solution (*e.g.*, Novák *et al.* 2004, Andreozzi *et al.* 2008, Bačík *et al.* 2012, 2013, Cempírek *et al.* 2013) as well as in Fe^{3+} -rich tourmalines (*e.g.*, Bačík *et al.* 2008, Bosi 2008, Bosi *et al.* 2010, Fareeduddin *et al.* 2010, Baksheev *et al.* 2011) indicating their extensive miscibility with uvite and feruvite endmembers.

Geological setting of the Mirošov pegmatite and its relations to anatectic pegmatites of the Moldanubian Zone

The shape and size of the Mirošov pegmatite body, its simple mineral assemblage, weak contact reactions, and close relationship to the metatects from surrounding amphibolites strongly suggest an anatectic origin. However, the crosscutting (brecciated) relationship of the pegmatite to the host calc-silicate rock and amphibolite, and locally sharp contacts exclude *in situ* anatexis; the pegmatite melt moved from its source at least tens to hundreds of meters, as seen in the amphibole-bearing

pegmatites cutting Fe-skarn at Vlastějovice (Novák *et al.* 2013). Common amphiboles, Ca-rich plagioclase, Ca-rich tourmaline, prehnite, and accessory epidote and titanite are also apparent indicators of external contamination, whereas the absence of more complex internal structure and pockets indicates a very primitive character for the pegmatite close to the metatects from the surrounding amphibolites.

Similar simple anatectic pegmatites are quite common in migmatized areas of the Moldanubian Zone and in particular in the Strážek Unit (Novák 2005, Novák *et al.* 1990, 2013, Cempírek *et al.* 2010). They typically exhibit a small thickness of pegmatite bodies (~0.05 to ~2 m), more or less simple internal structure, and commonly concordant relations to their gneissic host rocks; nevertheless, they are compositionally highly variable:

(1) Contaminated pegmatites cutting Ca-rich rocks such as calcite marble, Fe-skarn, and amphibolite contain common Ca-rich dravite (Povondra & Novák 1986) and Ca-rich schorl to feruvite (Novák *et al.* 2013), as well as minerals of the axinite group (Filip *et al.* 2006b) and amphiboles. These pegmatites are similar to the Mirošov pegmatite in size, internal structure, and mineralogy, except for Vlastějovice, where axinite and tourmaline are rare and fluorite very common,

indicating high activity of F and low activity of B at this particular locality (Novák *et al.* 2013).

(2) Contaminated pegmatites cutting Mg-rich rocks such as serpentinites (*e.g.*, Černý 1958, Novák 2005) are quite common as well. Dravite and uvite are typical tourmalines along with common phlogopite and rare amphibole (Prokop *et al.* 2013). Primary assemblages are often overprinted by strong hydrothermal alterations producing prehnite, chlorites, clay minerals, and zeolites (Černý & Povondra 1965a,b, Prokop *et al.* 2013).

(3) Mildly to moderately peraluminous pegmatites from migmatized gneisses and granulites with abundant muscovite, locally common andalusite and tourmaline (oxy-schorl, schorl, oxy-dravite, foitite, magnesio-foitite; Povondra 1981, Novák *et al.* 2004, Gadas *et al.* 2012), and characterized by pockets lined with crystals of smoky quartz, feldspars, muscovite, and tourmaline. They are common in the Strážek Unit (Gadas *et al.* 2012) and they are distinct in more complex internal structure, including common pockets and absence of external contamination. The closest localities are situated only hundreds of meters from the Mirošov pegmatite.

(4) Strongly peraluminous pegmatites with abundant muscovite, locally common kyanite, and rare staurolite are common, in particular along the northeastern-most margin of the Moldanubian Zone. A high B activity is documented by abundant Al-rich oxy-schorl, oxy-dravite, and olenite (Cempírek *et al.* 2006, Cempírek & Novák 2006) associated with common dumortierite (Cempírek & Novák 2006) and rather rare grandierite, werdingite, and boralsilite (Cempírek *et al.* 2010). They are similar to the Mirošov pegmatite in size and simple internal structure, but they do not show any features of contamination from the host—commonly peraluminous HT-HP/MP granulitic rocks.

Comparing accessory minerals from the individual types of simple anatectic pegmatites, we found some similarities: fluor-apatite and Ti-rich minerals (ilmenite, rutile, titanite; Novák *et al.* 1990, Černý *et al.* 2001, Gadas *et al.* 2012) are common, and As-rich minerals (löllingite, arsenopyrite > stibarsen) and rare W-bearing oxide minerals (Cempírek & Novák 2006, Cempírek *et al.* 2010, Fuksová *et al.* 2011, Gadas *et al.* 2012) are typical in most pegmatite types. Consequently, the anatectic pegmatites of the Moldanubian Zone and Strážek Unit in particular display similar features: (1) geological: small thickness, commonly concordant relations to host rocks; and (2) geochemical/mineralogical: common tourmaline and other B-rich minerals, similar accessory minerals disregarding the different degrees of external Ca- and/or Mg-contamination. The primitive geochemical/mineralogical features and geological setting support an anatectic origin for the pegmatite melts; however, the absence of restites at direct contacts, the locally discordant setting of the pegmatite bodies, and evident external contamination of some pegmatites

TABLE 7. SELECTED BOND LENGTHS (Å) IN TOURMALINE TU2 FROM MIROŠOV

X–O2	x3	2.5242 (15)
X–O5	x3	2.6920 (11)
X–O4	x3	<u>2.7640 (12)</u>
<X–O>		2.6601 Å
Y–O1		1.9993 (16)
Y–O2	x2	2.0468 (9)
Y–O3	x2	2.2180 (12)
Y–O6		<u>2.0383 (8)</u>
<Y–O>		2.0945 Å
Z–O3		1.9826 (6)
Z–O6		1.8909 (9)
Z–O7 ⁱ		1.9040 (8)
Z–O7		1.9756 (8)
Z–O8 ⁱ		1.9017 (8)
Z–O8		<u>1.9344 (8)</u>
<Z–O>		1.9315 Å
T–O4		1.6317 (5)
T–O5		1.6494 (6)
T–O6		1.6047 (10)
T–O7		<u>1.6063 (7)</u>
<T–O>		1.6230 Å
B–O2		1.3788 (18)
B–O8	x2	<u>1.3765 (10)</u>
<B–O>		1.3773 Å

Symmetry codes: (i) $-y+2/3$, $x-y+1/3$, $z+1/3$.

indicate that the melts were not generated *in situ* but were transported from their sources tens to hundreds of meters at least.

Comparison of tourmaline compositions from simple (anatectic) pegmatites of the Moldanubian Zone

Tourmalines from simple anatectic pegmatites of the Moldanubian Zone are highly variable with regard to their host rocks, degree of contamination, and crustal position (see above). Strongly peraluminous pegmatites (4) involving rather deep-seated dumortierite-bearing pegmatites and borosilicate veins in granulite from Horní Bory with Al-rich tourmalines (oxy-schorl, olenite; Cempírek & Novák 2006, Cempírek *et al.* 2006, 2010) are compositionally very distinct from the Ca-rich schorl to feruvite at Mirošov; hence, they will not be discussed in detail.

Anatectic pegmatites with pockets (3) abundant in the Strážek Unit are characterized by common tourmaline present in several distinct morphological and paragenetic types: *e.g.*, irregular aggregates, quartz-tourmaline graphic intergrowths, and prismatic crystals in massive pegmatite and crystals of their aggregates with variable size and morphology in pockets (Gadas *et al.* 2012). Tourmalines from Mirošov significantly differ, forming interstitial networks between grains of feldspars, quartz, and amphibole, and graphic intergrowths with quartz in central parts of the pegmatite. Regarding the chemical compositions of tourmaline from pocket pegmatites (3) and from Mirošov, they both show low to negligible contents of Li, F, Cr, and V as well as Mn (0.00–0.04 *apfu*), and moderately elevated contents of Ti (0.01–0.14 and 0.04–0.24 *apfu*, respectively). Thus, the essential differences include lower contents of Al (4.77–5.77 and 6.28–7.19 *apfu*) and higher Mg (0.46–1.92 and 0.01–1.58 *apfu*) in tourmalines from Mirošov and the pocket pegmatites, respectively. In addition, strong Ca-enrichment in tourmaline from Mirošov (0.37–0.58 *apfu*) is evident relative to the pocket pegmatites with ≤ 0.15 *apfu* Ca.

Tourmalines from simple contaminated pegmatites (1) and (2) of the Moldanubian Zone are also highly variable, but rather similar in low to moderate $Al_{tot} = 5.10$ –6.43 *apfu*, moderate to high Ca = 0.14–0.56 *apfu*, and low X-site vacancy = 0–0.10 *pfu*. Most analyses also show low F, ≤ 0.10 *apfu*. However, they are quite variable in $Mg/(Mg + Fe_{tot})$; Mg-rich tourmalines are typical for the pegmatites enclosed in serpentinites (Prokop *et al.* 2013, unpubl. data of MN) or calcite marbles (Povondra & Novák 1986), whereas Fe-rich tourmalines occur in pegmatites cutting Fe-skarn (Novák *et al.* 2013) or calc silicate rock (Mirošov, this work). Hence, the role of external contamination is crucial and the composition of the Mg-rich host rock is more pronounced in tourmaline compositions. At Vlastějovice, the Fe-skarn has $Fe \gg Mg$, hence, very

high Fe in tourmaline is feasible. However, Fe^{2+}/Fe^{3+} in the individual tourmalines is mostly not known.

Comparison of Ca,Fe-rich tourmalines from various geological environments

Compositions of tourmaline from the individual paragenetic types/localities vary from rather homogeneous (Manning 1991, Selway *et al.* 1998) to highly heterogeneous (Selway *et al.* 2000, Novák *et al.* 2013, this work); however, it is necessary to take into account the variable number of analyses and examined samples at the individual localities. The chemical compositions of the feruvitic tourmalines are characterized by low X-site vacancies that decrease with increasing Ca content (≤ 0.64 *apfu*; Fig. 6b); feruvite from Mirošov has the highest Ca content in pegmatites (≤ 0.58 *apfu*). Tourmalines show high variability in Mg and Fe; the highest Fe_{tot} content (≤ 3.21 *apfu*) was found in Ca-rich schorl from Vlastějovice (Novák *et al.* 2013). This is in contrast to feruvitic tourmalines of hydrothermal origin showing relatively high Mg contents projecting analyses close to the uvite/feruvite and dravite/schorl boundary, including the feruvite type locality (Grice & Robinson 1989; Fig. 6a). The variable contents of Al (mostly < 6 *apfu*) are comparable in all three paragenetic groups, but differ significantly within some individual occurrences (Fig. 6d). All feruvitic tourmalines are significantly Ti-enriched (≤ 0.36 *apfu*; Jiang *et al.* 1996), and Ti contents slightly positively correlate with Ca contents (Fig. 6c). Very low contents of Mn are typical for all feruvitic tourmalines as well. Slightly elevated contents were observed only in pegmatites (≤ 0.07 *apfu* for Vlastějovice; Novák *et al.* 2013) and exceptionally in Mirošov ≤ 0.07 *apfu*. Feruvitic tourmalines from pegmatite exocontacts show the highest contents of F (≤ 0.60 *apfu*; Selway *et al.* 1998, 2000) along with moderately F-enriched tourmalines from the Vlastějovice pegmatite (≤ 0.36 *apfu*); F contents in most of the hydrothermal feruvitic tourmalines are very low, as well as at Mirošov (≤ 0.11 *apfu*).

Feruvitic tourmaline from Mirošov contains 45% of Fe^{3+} from Fe_{tot} obtained by Mössbauer spectroscopy (Table 3) and supported by single-crystal XRD data. Due to the lack of spectroscopic studies, we cannot compare other feruvitic tourmalines, except for feruvite from the type locality (Grice & Robinson 1989, Grice & Ercit 1993) with $\sim 19\%$ of Fe^{3+} from Fe_{tot} calculated by stoichiometry and from single-crystal XRD. Similarly, very low contents of Li found in tourmaline from Mirošov as determined using LA-ICP-MS are in contrast with Li-enriched feruvitic tourmalines from exocontacts of Li-rich pegmatites (≤ 0.31 *apfu*); however, the Li contents were calculated from stoichiometry (Selway *et al.* 1998, 2000) and they are very likely significantly overestimated.

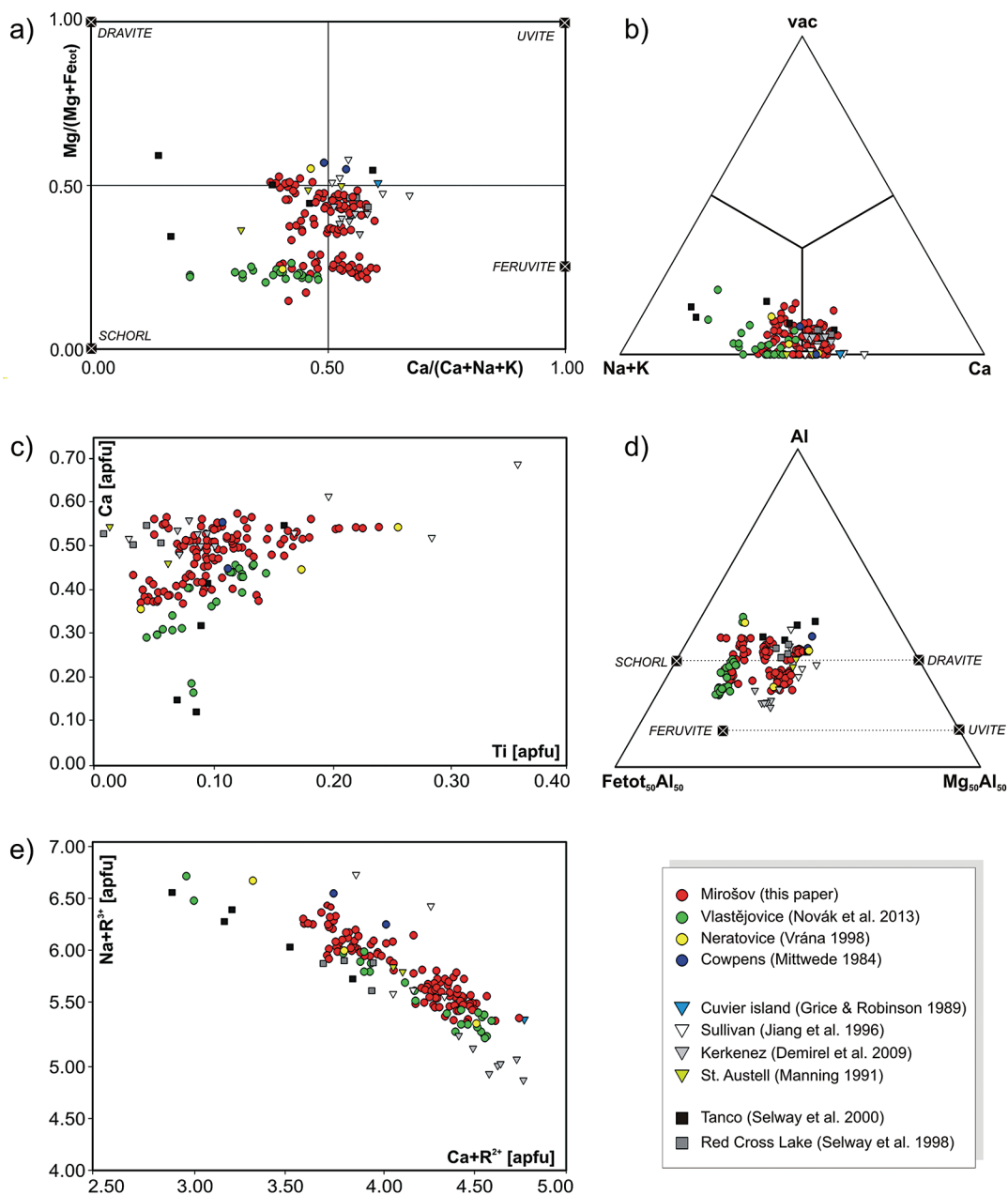


FIG. 6. Plots and triangular diagrams showing the comparison of tourmalines from Mirošov (except of the type TU3) and other Ca,Fe rich tourmalines of different paragenetic types. (a) X_{Mg}/X_{Ca} plot; (b) diagram of X-site occupancy; (c) Ca/Ti plot; (d) diagram of Y-site occupancy; (e) Na+R³⁺/Ca+R²⁺ plot. Circles = pegmatitic occurrences; triangles = hydrothermal occurrences; squares = tourmalines from pegmatite exocontacts. Endmember projections of schorl, dravite, uvite, and feruvite are also shown in (a) and (d).

Each individual paragenetic group of feruvitic tourmalines is characterized by some specific chemical composition or enrichment by specific element; however, in general, their compositions are rather similar (Fig. 6). The chemical composition of tourmaline from individual occurrences reflects its geochemical environment (melt or fluids + contamination from host rocks), P-T conditions, and crystal-structural constraints (e.g., Hawthorne 2002, Bosi 2011); however, Ca (≤ 0.64 apfu) is low relative to uivite with up to ~ 0.85 apfu Ca (cf. Fantini *et al.* 2013). The formation of feruvite requires specific geochemical conditions with high activities of Ca and Fe, but rather low Mg, a rare geological environment in nature. This explains the scarcity of feruvite relative to uivite.

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