

Chemical composition and crystal structure refinement of schorl from the Lundazi pegmatite field, Zambia

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Abstract. Present work characterizes tourmaline from one of the major pegmatite fields in Zambia – the Lundazi pegmatite belt.

Microprobe analysis gave (wt%): SiO₂ 34.65, TiO₂ 0.85, Al₂O₃ 29.80, Fe₂O₃ 4.94, FeO 9.47, MnO 0.29, MgO 4.06, Li₂O < 0.01, CaO 0.59, Na₂O 2.38, K₂O 0.08, F 0.32, H₂O+ 3.24, B₂O₃ 10.32, O=F –0.14, totalling 100.45. The empirical formula, calculated on the basis of 31 (O, OH, F) per formula unit gives: (Na_{0.78}Ca_{0.11}K_{0.02}□_{0.09})_{Σ1.00} (Fe²⁺_{1.33}Fe³⁺_{0.63}Mg_{0.61}Ti_{0.11}Mn_{0.04}□_{0.12})_{Σ3.00} (Al_{5.59}Mg²⁺_{0.41})_{Σ6.00} [(Si_{5.84}Al_{0.16})_{Σ6.00}O_{18.00}] (BO₃)_{3.00} (OH)_{3.00} [(OH)_{0.64}O_{0.19}F_{0.17}]_{Σ1.00} resulting in simplified formula: Na(Fe²⁺,Fe³⁺,Mg)₃(Al,Mg)₆(Si₆O₁₈)(BO₃)₃(OH)₃ (OH, O, F). Analysis of Mössbauer spectra confirms both Fe²⁺ and Fe³⁺ in the Y site; Fe³⁺/Fe²⁺ is 0.47. The water was determinate using Karl Fischer titration, B₂O₃ was calculated to stoichiometry. Refined crystal structure data (atomic coordinates, inter-atomic distances and angles) are in agreement with data for schorl. Mean polyhedron distances are (Å): X-O 2.646, Y-O 2.078, Z-O 1.939, Si-O 1.644, B1-O 1.382. The refined unit-cell parameters are: *a* = 15.9856 (2), *c* = 7.1892 (1) Å, *V* = 1591.00(4) Å³, space group is *R3m*, *Z*=3. *D*_m = 3.18(1) g/cm³, *D*_x = 3.195(2) g/cm³. Streak is light grey, lustre is glassy. Pleochroism in powder mounts: ε = light brownish red, ω = dark bluish grey (thin fragments), ε = strong brownish red, ω = opaque (thick fragments). The studied sample belongs to hydroxy-tourmaline subgroup with 19 atomic % of oxy subgroup (Fe³⁺/Fe²⁺ = 0.47 in the Y site and ratio O/(OH⁻) = 0.30 in the W site).

Abstrakt. Práce charakterizuje turmalín z jedné z hlavních pegmatitových lokalit Zambie – pegmatitového pásma Lundazi.

Lokální bodová analýza (LAREM) poskytla chemickou analýzu (hm.%): SiO₂ 34.65, TiO₂ 0.85, Al₂O₃ 29.80, Fe₂O₃ 4.94, FeO 9.47, MnO 0.29, MgO 4.06, Li₂O <0.01, CaO 0.59, Na₂O 2.38, K₂O 0.08, F 0.32, H₂O+ 3.24, B₂O₃ 10.32, O=F –0.14, suma 100.45. Empirický vzorec rozpočtený na 31 (O, OH, F) atomů na vzorcovou jednotku poskytuje: (Na_{0.78}Ca_{0.11}K_{0.02}□_{0.09})_{Σ1.00} (Fe²⁺_{1.33}Fe³⁺_{0.63}Mg_{0.61}Ti_{0.11}Mn_{0.04}□_{0.12})_{Σ3.00} (Al_{5.59}Mg²⁺_{0.41})_{Σ6.00} [(Si_{5.84}Al_{0.16})_{Σ6.00}O_{18.00}] (BO₃)_{3.00} (OH)_{3.00} [(OH)_{0.64}O_{0.19}F_{0.17}]_{Σ1.00}, zjednodušeně: Na(Fe²⁺,Fe³⁺,Mg)₃(Al,Mg)₆(Si₆O₁₈)(BO₃)₃(OH)₃ (OH, O,F). Analýza Mössbauerova spektra potvrdila Fe²⁺ a Fe³⁺ pouze v pozicích Y; vypočtený poměr Fe³⁺/Fe²⁺ je 0.47. Voda byla stanovena Karl Fischerovou titrací, B₂O₃ byl doložen ze stechiometrie. Zpřesněná data krystalové struktury (pozice atomů, meziatomové vzdálenosti a úhly) jsou v dobré shodě s daty pro skoryl. Střední vzdálenosti polyedrů jsou (Å): X-O 2.646, Y-O 2.078, Z-O 1.939, Si-O 1.644, B1-O 1.382. Zpřesněné parametry základní cely jsou: *a* = 15.9856 (2), *c* = 7.1892 (1) Å, *V* = 1591.00(4) Å³, s.g. *R3m*, *Z* = 3. *D*_m = 3.18(1) g/cm³, *D*_x = 3.195(2) g/cm³. Vryp je světle šedý, lom skelný. Pleochroismus práškového preparátu: ε = světle hnědavě červená, ω = tmavě modravě šedá (tenké fragmenty), ε = silně hnědavě červená, ω = opakní (silné fragmenty). Studovaný vzorek patří do podskupiny hydroxy turmalínů s 19 atom. % oxysložky.

Key words: pegmatite, tourmaline, schorl, chemical composition, crystal structure, refinement, cell parameters, pleochroism, Mössbauer spectroscopy, XRD powder diffraction