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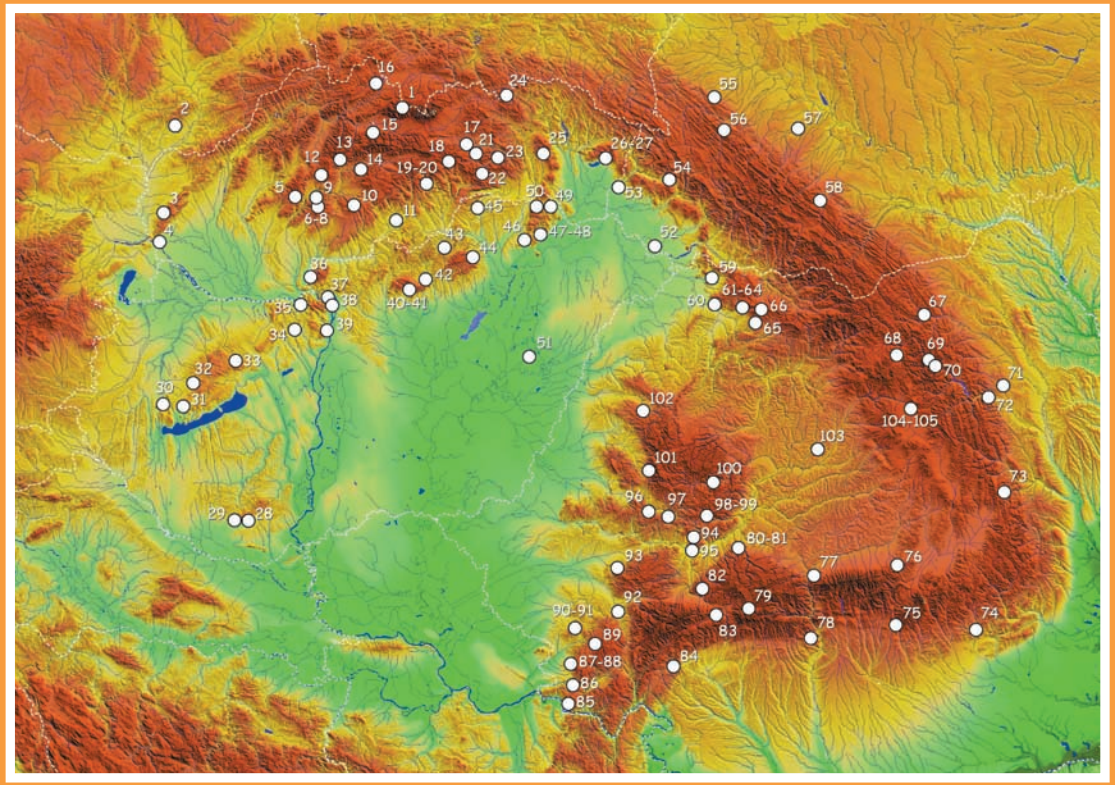

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Chemical classification of tourmalines using the RHA method

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A representation of the mineral chemistry for the tourmaline group needs a series of ternary diagrams (up to 16!), any of which, however, can't clearly display the complexity of even one mineral species [1]. We compiled a collection of 788 chemical analyses of natural tourmalines from 33 occurrences. These chemical data were classified using the PETROS program (author S.Moshkin), based on a method developed by T. Petrov [2], and as a result, we obtained the set of ordered RHA data.

R, the rank formula, is a sequence of chemical elements symbols of any analysis ordered on decreasing of their atomic %. En, the information entropy, is the characteristic reflecting complexity of the composition. An, the anentropy, reflects the purity of analysis. The diversity of our tourmalines compositions is represented in uniform hierarchical RHA table, where rank formulae are ordered as in dictionaries according to the number of elements in the Periodic Table. Our RHA-data can be searched in Internet by name: RHA language-method with cited files RHA-Tourmaline-2005.rar, RHA-Tur-Groups-2005.rar and Help_Turm-En on web-site: http://geology.pu.ru/.

Examples of rank formulae (R) for main tourmaline species are shown in Table 1 (elements in brackets can exchange in their rank position):

Table 1: Rank formulas of main tourmaline species

OAlSi(HB)**Li**(**Na**F...)	elbaite
OAlSi(HB**Li**)(**Ca**FNa...)	liddicoatite
O(AlSi)(HB**Mg**)(**NaV**Ca)…	vanadiumdravite
O(AlSi)(HB**MgCr**Na)...	chromdarvite
O(AlSi)(HB)**Mg**(**Na**Fe)…	dravite
OAlSi(HB)(**MnNa**FLi...)	tsilaisite
O(AlSi)(HB**Fe**)(**Na**Mg…)	schorl

In isomorphic rows, the predominance of one element over next in rank formulas can be used for impartial distinguishing of different mineral species. For example: when Mg > Fe – dravites, Fe > Mg – schorls. Combination of bold element symbols point at species inside the tourmaline group. Our suggestions for tourmaline chemical classification in more detail were published in [3].

The RHA-method gives the possibility to allocate the simple and clear-cut groups of the basic mineral species and subspecies; to define them authentically; to search for analogues without preliminary identification of a mineral variety; to estimate the originality of compositions. The RHA-method expands opportunities for improving nomenclature of minerals.

The RHA Database can be integrated in uniform classification of all mineral and rock compositions.

[1] Hawthorne, F.C. & Henry, D.J. (1999) *Eur. J. Mineral.*, **11**, 201-215. [2] Petrov, T.G. (2008) *Otechestvennaya Geologiya*, **4**, 98-105 (in Russian). [3] Andriyanets-Buyko, A.A., et al. (2007) *Zap. Ross. Mineral. Obshchest.*, **136**, 26-41 (in Russian).

Manganoeudialyte, a new mineral from Poços de Caldas, Minas Gerais, Brazil

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Manganoeudialyte is a new mineral with ideal formula $Na_{14}Ca_6Mn_3Zr_3[Si_{26}O_{72}(OH)_2]Cl_2 \cdot 4H_2O$, from a khibinite from the northern edge ("Anel Norte") of the alkaline Poços de Caldas massif, Minas Gerais, Brazil. It is concentrated in cm-sized patches interstitial to the main minerals of the rock. Associated minerals are eudialyte, K-feldspar, nepheline, aegirine, analcime, sodalite, rinkite, lamprophyllite, astrophyllite, titanite, fluorite, and cancrinite. Color is pink to purple, streak is white, and luster is vitreous. It is transparent to translucent and is not fluorescent. Mohs hardness is between 5 and 6, tenacity is brittle. Measured density is 2.890 g/cm^3; the calculated density is 2.935 g/cm^3. Manganoeudialyte is uniaxial (+), ω = 1.603(2), ε = 1.608(2) (white light). It is nonpleochroic.

The chemical composition is (by WDS mode electron microprobe data, H_2O content determined by the Penfield method, wt.%): Na_2O 12.01, K_2O 0.59, CaO 10.70, MnO 3.51, SrO 3.00, FeO 2.72, Al_2O_3 0.41, La_2O_3 0.15, Ce_2O_3 0.12, SiO_2 48.70, TiO_2 0.47, ZrO_2 12.08, Nb_2O_5 1.21, HfO_2 0.25, F 0.08, Cl 0.99, H_2O 3.5, -O=(Cl,F) -0.26, total 100.23. The empirical formula based on (Si + Al + Zr + Ti + Hf + Nb) = 29 is: $H_{12.08}Na_{12.05}Sr_{0.90}K_{0.39}La_{0.03}Ce_{0.02}Ca_{5.93}(Mn_{1.54}Fe_{1.18})Zr_{3.03}Nb_{0.28}Al_{0.25}Hf_{0.04}Ti_{0.18}Si_{25.20}O_{79.40}Cl_{0.87}F_{0.13}$.

The crystal structure was solved on a single crystal to R = 0.033. The mineral is trigonal, $R3m$; a = 14.2418(1), c = 30.1143(3) Å, V = 5289.7(1) Å^3, Z = 3. The coordination numbers are 6 for Mn, and 5 for Fe. The distorted octahedron $[MnO_4(H_2O)_2]$ contains two types of H_2O molecules. The crystal chemical formula of manganoeudialyte is: $[Na_{11.93}Sr_{0.81}(H_3O)_{0.70}K_{0.39}Ce_{0.07}]_{\Sigma 13.90}Ca_6]$ $[^{VI}Mn_{1.56}{}^{V}Fe_{1.20}{}^{V}Na_{0.24}]_{\Sigma 3.00}$ $[Zr_3]$ $[^{IV}(Si_{0.38}Al_{0.25})^{VI}(Nb_{0.29}Zr_{0.08})]_{\Sigma 1.00}$ $[^{IV}Si_{0.81}{}^{VI}Ti_{0.19}]_{\Sigma 1.00}$ $[Si_{24}O_{72}]$ $[(OH)_2][(H_2O)_{3.55}Cl_{0.88}(OH)_{0.84}O_{0.40}$ $F_{0.13}]_{\Sigma 5.80}$. The strongest reflection peaks of the powder diffraction pattern [d, Å (I, %) (hkl)] are: 6.421 (37) (104), 4.329 (30) (205), 3.526 (46) (027), 3.218 (100) (208), 3.023 (25) (042), 1.609 (77) (4.1.15), 1.605 (41) (4.0.16). IR spectrum shows that the mineral contains at least two locally different types of water molecules (the bands at 1620 and 1677 cm^{-1}) and the polyhedra $[Fe^{2+}O_5]$ (the band at 529 cm^{-1}). The new mineral species has been approved by the CNMNC (IMA 2009-039).