

Article

Who Is Who in the Eudialyte Group: A New Algorithm for the Express Allocation of a Mineral Name Based on the Chemical Composition

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Abstract: Eudialyte-group minerals (EGMs) are Na-Ca zirconosilicates typical for peralkaline plutonic rocks. In the zeolite-like crystal structure of these minerals, there are many sites of different volumes and configurations, and therefore EGMs can include up to one-third of the periodic table. Although there are preferred sites for many elements in the crystal structure of eudialyte-group minerals, the same element can appear in several sites. In addition, many sites may be partially or fully vacant. Currently, 30 mineral species are established in the eudialyte group. However, this diversity is, in fact, limited to holotype specimens. To name any mineral from the eudialyte group, you need to solve its crystal structure and compare it with holotypes. Meanwhile, the composition (and, therefore, the name) of any mineral of the eudialyte group is an excellent indicator of the composition of the mineral-forming media, which is very important to petrological and mineralogical studies. In this article, we propose a diagnostic scheme for minerals of the eudialyte group, based only on the chemical composition. The scheme includes five consecutive steps, each of which evaluates the content of a species-forming element (or the sum of such elements). This scheme can be supplemented by new members without changing its hierarchical structure.

Keywords: eudialyte group; systematic; classification; diagnostics; mineral; peralkaline rocks



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1. Introduction

Eudialyte-group minerals (EGMs) are alkaline zirconium-calcium silicates that accommodate many different elements in their complex zeolite-like structure. In addition to Si, Na, Ca, and Zr EGMs comprise significant amounts of Fe, Mn, REE, Y, Nb, Hf, Ti, K, Sr, and Cl, F, H₂O and OH groups [1–4]. The crystal structures of EGMs are based on a heteropolyhedral framework (Figure 1) formed by three types of layers: the T-layer containing three- and nine-membered rings of SiO₄-tetrahedra [(Si₃O₉) and (Si₉O₂₇), respectively]; the M-layer represented by six-membered [M(1)₆O₂₄] rings of edge-shared M(1)O₆-octahedra; and the Z-layer of isolated ZO₆ octahedra. These layers alternate along the *c* parameter in the ... |TMTZ| ... sequence (the thickness of the TZTM fragment is ~10 Å), and according to an *R*-lattice they form “12-layer” eudialytes (*a*~14.2 Å, *c*~30 Å) [5]. In “24-layer” “megaeudialytes”, a doubling of the *c*-period of the unit cell (*a*~14.2 Å, *c*~60 Å) is observed.

The eudialyte group combines 30 mineral species and a wide range of their varieties have been described. The crystal chemical formula of EGMs (derived from the IMA approved formula [2]) can be written as (*Z* = 3):

$$\{N(1)_3N(2)_3N(3)_3N(4)_3N(5)_3\}\{[M(1a)_3M(1b)_3]_3M(2)_3M(3)_3M(4)_3Z_3[Si_{24}O_{72}]O_{0-6}\}X(1)X(2),$$

where

$$N(1-5) = \text{Na, H}_3\text{O}^+, \text{K, Sr, REE, Y, Ba, Mn, Ca, } \square \text{ (vacancy);}$$

$M(1) = \text{Ca, Mn, REE, Na, Fe};$
 $M(2) = \text{IV,VFe}^{2+}, \text{V,VIFe}^{3+}, \text{V,VI}^{2+}, \text{V,VI}^{3+}, \text{V,VI}^{4+};$
 $M(3) \text{ and } M(4) = \text{IV,Si, VI,Nb, VI,Ti, VI,W}^{6+}, \square;$
 $Z = \text{Zr, Ti, Nb};$
 $\emptyset = \text{O, (OH)};$
 $X = \text{Cl, F, S}^{2-}, \text{H}_2\text{O, CO}_3, \text{and SO}_4.$

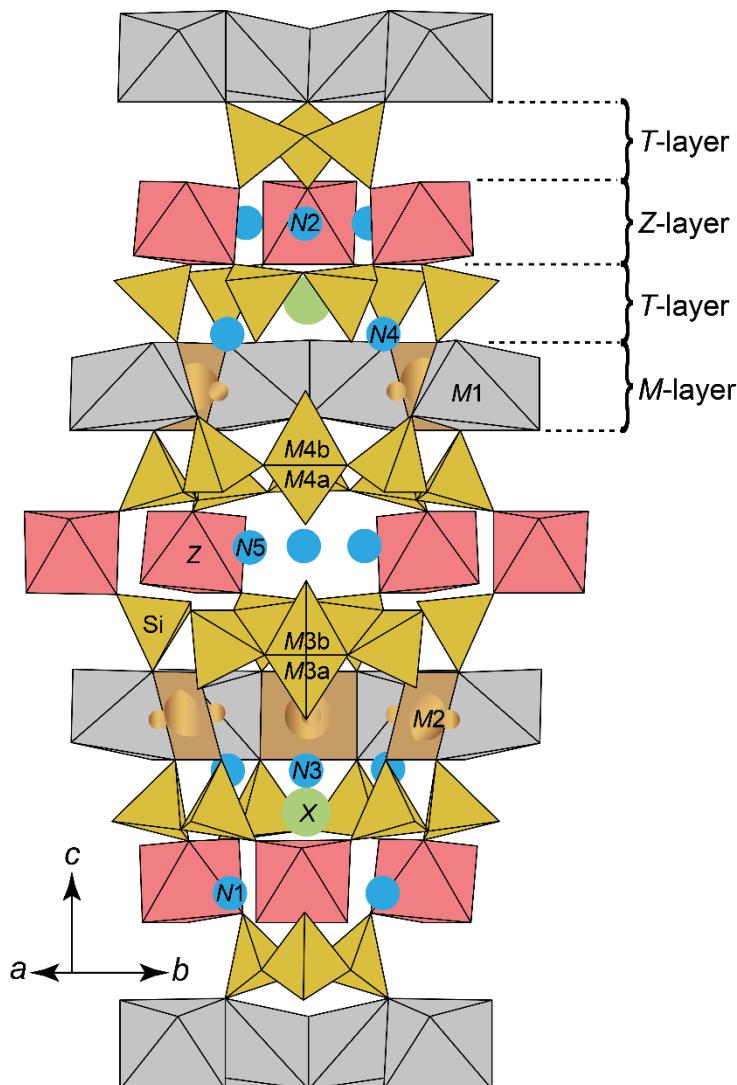


Figure 1. The general view of crystal structure of “12-layer” EGMs.

The $M(3)$ and $M(4)$ sites are located at the centers of the $(\text{Si}_9\text{O}_{27})$ rings and are predominantly occupied by Si, Nb, W, and some other components or can be partly vacant. In addition, the $M(2)$ site is located at $M(2)\text{O}_4\emptyset_n$ -polyhedra ($n = 0–2$) between the octahedral six-membered rings. The $M(2–4)$ sites form microregions of split “subsites” with close distance to each other. These “subsites” can differ by their chemical composition and/or coordinational environment [6]. The large cavities of the zeolite-like framework are filled by extraframework cations and water molecules located at $N(1)–N(5)$ sites.

The principles of nomenclature of the eudialyte-group minerals have been developed by the Eudialyte Nomenclature Subcommittee established by the Commission on New Minerals and Mineral Names of the International Mineralogical Association [2]. The following nomenclature schemes have been tested:

- (1) Linnean biological principle;

- (2) Hierarchical system with root names modified by using the modifiers and Levinson suffixes;
- (3) A unique-name system using the modifiers.

Conventional unique names with a maximum of one cation prefix are recommended for the eudialyte-group minerals, and this prefix should refer to the M(2) site. As in other groups of minerals, a new mineral in the eudialyte group is considered to be one in which at least one structural position is occupied by a different chemical element than in other minerals with a similar structure. Empirical and CNMNC formulas of the IMA-approved members of the eudialyte group are presented in Table 1, and site occupancies are shown in Table 2.

Table 1. Empirical and corresponding CNMNC formulas of the of the IMA-approved members of the eudialyte group.

Mineral	Empirical Formula */IMA Formula	Ref.
Alluaivite	$(Na_{17.47}K_{0.12}La_{0.03}Ce_{0.14}Sr_{0.28}Ba_{0.11})(Ca_{4.46}Mn_{1.47})Si_{25.85}O_{73.26}$ $(Ti_{2.18}Zr_{0.05}Nb_{0.85})Cl_{0.66}\cdot 2.75H_2O$ $Na_{19}(Ca,Mn^{2+})_6(Ti,Nb)_3Si_{26}O_{74}Cl\cdot 2H_2O$	[7]
Andrianovite	$Na_{12.09}(K_{1.40}Sr_{0.97}REE_{0.60}Ba_{0.04})\Sigma 3.01(Ca_{5.90}Y_{0.08})\Sigma 5.98(Mn_{1.81}Fe^{2+}1.19)\Sigma 2.90(Zr_{2.96}Hf_{0.04})\Sigma 3.0$ $(Nb_{0.69}Si_{0.27}Ti_{0.05}Al_{0.01})\Sigma 1.02(Si_{25}O_{73})[O_{2.14}(OH)_{0.52}]\Sigma 2.66[(H_2O)_{1.30}(CO_3)_{0.42}Cl_{0.28}]\Sigma 2.0$ $Na_{12}(K,Sr,Ce)_3Ca_6Mn_3Zr_3Nb(Si_{25}O_{73})(O,H_2O,OH)_5$	[8]
Aqualite	$[(H_3O)_{7.94}Na_{2.74}K_{1.20}Sr_{0.49}Ba_{0.46}Fe_{0.23}Mn_{0.12}]\Sigma 13.18(Ca_{5.79}REE_{0.19})\Sigma 5.98(Zr_{2.92}Ti_{0.08})\Sigma 3.0$ $(Si_{25.57}Ti_{0.21}Al_{0.19}Nb_{0.03})\Sigma 26.01[O_{66.46}(OH)_{5.54}]\Sigma 72.01[(OH)_{2.77}Cl_{1.23}]\Sigma 4.0$ $(H_3O)_8(Na,K,Sr)_5Ca_6Zr_3Si_{26}O_{66}(OH)_9Cl$	[9]
Carbokentbrooksite	$(Na_{9.43}Ca_{0.90}K_{0.36})\Sigma 10.69[Na_{1.39}(Ce_{0.60}La_{0.36}Nd_{0.15}Pr_{0.05})\Sigma 1.16Sr_{0.45}]\Sigma 3(Ca_{5.34}Mn_{0.54}Y_{0.12})\Sigma 6$ $(Mn_{1.98}Fe_{1.02})\Sigma 3(Zr_{2.96}Ti_{0.04})\Sigma 3(Nb_{0.88}Ti_{0.13})\Sigma 1.01Si_{25}H_{4.32}O_{77.64}(CO_3)_{0.58}Cl_{0.27}$ $(Na,\square)_{12}(Na,Ce)_3Ca_6Mn_3Zr_3NbSi_{25}O_{73}(OH)_3(CO_3)\cdot H_2O$	[10]
Davinciite	$(Na_{11.75}Sr_{0.29}Ba_{0.03})\Sigma 12.07(K_{2.28}Na_{0.72})\Sigma 3Ca_{5.99}(Fe_{2.26}Mn_{0.16})\Sigma 2.42(Zr_{2.80}Ti_{0.15}Hf_{0.03}Nb_{0.02})\Sigma 3$ $(Si_{1.96}Al_{0.04})\Sigma 2[Si_3O_9]_2[Si_9O_{27}]_2[(OH)_{1.42}O_{0.58}]\Sigma 2[Cl_{1.62}(H_2O)_{0.38}]\Sigma 2\cdot 0.48H_2O$ $Na_{12}K_3Ca_6Fe^{2+}3Zr_3(Si_{26}O_{73}OH)Cl_2$	[11]
Dualite	$(Na_{29.79}Ba_{0.1}K_{0.10})\Sigma 30(Ca_{8.55}Na_{1.39}REE_{1.27}Sr_{0.79})\Sigma 12(Na_{3.01}Mn_{1.35}Ti_{0.77})\Sigma 6(Zr_{2.61}Nb_{0.39})\Sigma 3$ $(Ti_{2.52}Nb_{0.48})\Sigma 3(Mn_{0.82}Si_{0.18})\Sigma 1(Si_{50.77}Al_{0.23})\Sigma 1O_{144}[(OH)_{6.54}(H_2O)_{1.34}Cl_{0.98}]\Sigma 8.86$ $Na_{30}(Ca,Na,Ce,Sr)_{12}(Na,Mn,Fe,Ti)_6Zr_3Ti_3MnSi_{51}O_{144}(OH,H_2O,Cl)_9$	[12]
Eudialyte	$Na_{15}Ca_6Fe_3Zr_3Si(Si_{25}O_{73})(O,OH,H_2O)_3(Cl,OH)_2$	[13]
Feklichevite	$Na_{10.85}Ca_{9.15}REE_{0.08}Fe_{2.00}Mn_{0.25}Ti_{0.05}Zr_{3.05}Hf_{0.04}Nb_{0.62}Si_{25.61}O_{75.89}Cl_{0.21}$ $Na_{11}Ca_9(Fe^{3+},Fe^{2+})_2Zr_3Nb(Si_{25}O_{73})(OH,H_2O,Cl,O)_5$	[14]
Fengchengite	$[(Na_{3.00}Na_{3.00})\Sigma 6.00(Na_{5.28}K_{0.33}\square_{0.39})]\Sigma 12.00(\square_{2.71}Sr_{0.20}REE_{0.09})\Sigma 3.00(Ca_{4.80}Sr_{0.82}Fe^{2+}0.29$ $Mg_{0.05}Mn_{0.04})\Sigma 6.00(Fe^{3+}2.25Mn_{0.35}Cr_{0.08}\square_{0.32})\Sigma 3.00(Zr_{2.86}Ti_{0.09}Nb_{0.05})\Sigma 3.00(Si_{0.87}Ti_{0.05}\square_{0.08})\Sigma 1.00$ $Si(Si_{24.00}O_{73.00})[(H_2O)_{2.93}(OH)_{0.07}]\Sigma 3.00[(OH)_{1.04}Cl_{0.96}]\Sigma 2.00$ $Na_{12}\square_3Ca_6Fe^{3+}3Zr_3Si(Si_{25}O_{73})(H_2O)_3(OH)_2$	[15]
Ferrokentbrooksite	$(Na_{13.05}REE_{0.99}K_{0.32}Ca_{0.23}Sr_{0.15})_{14.74}(Ca_{4.59}Mn_{1.24}Y_{0.17})_6(Fe_{2.39}Mn_{0.61})_3$ $(Zr_{3.00}Ti_{0.04}Hf_{0.03})_{3.07}(Nb_{0.64}Si_{0.23}Zr_{0.07}Ta_{0.02})_{0.96}(Si_{24.93}Al_{0.07})_{25}O_{73}$ $(O,OH,H_2O)_{2.47}(Cl_{0.89}F_{0.71}OH_{0.40})_2$ $Na_{15}Ca_6Fe^{2+}3Zr_3Nb(Si_{25}O_{73})(O,OH,H_2O)_3(F,Cl)_2$	[16]
Georgbarsanovite	$(Na_{11.74}K_{0.24})\Sigma 11.97(Mn_{1.19}Sr_{0.71}REE_{0.63}Ca_{0.30}Y_{0.13}Ba_{0.03})\Sigma 2.99Ca_6(Fe^{2+}2.55Zr_{0.23}Ti_{0.05}Hf_{0.04})\Sigma 2.87$ $Zr_3Nb_{0.92}Si_{25.25}O_{76.48}Cl_{1.11}F_{0.61}\cdot 0.88H_2O$ $Na_{12}(Mn,Sr,REE)_3Ca_6Fe^{2+}3Zr_3NbSi_{25}O_{76}Cl_2\cdot H_2O$	[17]
Golyshevite	$(Na_{9.02}Ca_{0.43}K_{0.30})\Sigma 9.75Ca_3(Ca_{5.92}Ce_{0.05}La_{0.03})\Sigma 6.00Fe^{3+}1.69Fe^{2+}0.50Mn_{0.29}Zr_{2.97}$ $(Nb_{0.60}Si_{0.66}Al_{0.08})Si_{24}O_{72}(OH)_{2.37}(CO_3)_{1.05}Cl_{0.21}\cdot 1.01H_2O$ $Na_{10}Ca_9Zr_3Fe_2SiNb(Si_3O_9)_2(Si_9O_{27})_2(OH)_3(CO_3)\cdot H_2O$	[18]

Table 1. Cont.

Mineral	Empirical Formula */IMA Formula	Ref.
Ikranite	$\text{Na}_{7.56}(\text{H}_3\text{O})_{6.64}\text{K}_{0.27}\text{Ca}_{3.31}\text{Sr}_{0.46}\text{Ce}_{0.27}\text{La}_{0.11}\text{Nd}_{0.03}\text{Mn}_{1.41}\text{Fe}^{2+}_{0.16}\text{Fe}^{3+}_{1.77}\text{Zr}_{3.33}\text{Ti}_{0.14}\text{Hf}_{0.04}$ $\text{Nb}_{0.06}\text{Si}_{24}\text{O}_{72}\text{Cl}_{0.74}\cdot 2.64\text{H}_2\text{O}$ $(\text{Na},\text{H}_3\text{O})_{15}(\text{Ca},\text{Mn},\text{REE})_6\text{Fe}^{3+}_2\text{Zr}_3\text{Si}_{24}\text{O}_{66}(\text{O},\text{OH})_6\text{Cl}\cdot \text{nH}_2\text{O}$	[19]
Ilyukhinite	$\text{H}_{36.04}(\text{Na}_{3.82}\text{K}_{0.20})(\text{Ca}_{5.65}\text{Ce}_{0.22}\text{La}_{0.14}\text{Nd}_{0.07})(\text{Mn}_{1.285}\text{Fe}_{0.48})(\text{Zr}_{2.645}\text{Ti}_{0.34})$ $\text{Nb}_{0.31}\text{Si}_{25.41}\text{S}_{0.42}\text{Cl}_{0.23}\text{O}_{86.82}$ $(\text{H}_3\text{O},\text{Na})_{14}\text{Ca}_6\text{Mn}_2\text{Zr}_3\text{Si}_{26}\text{O}_{72}(\text{OH})_2\cdot 3\text{H}_2\text{O}$	[20]
Johnsenite-(Ce)	$\text{Na}_{11.74}([\text{Ce}_{0.64}\text{La}_{0.33}\text{Dy}_{0.03}]_{\Sigma 1.00}\text{Sr}_{0.54}\text{Ca}_{0.51}\text{Y}_{0.22}\text{K}_{0.19}\text{Hf}_{0.01})_{\Sigma 2.47}(\text{Ca}_{5.06}$ $[\text{Pr}_{0.24}\text{Nd}_{0.18}\text{Gd}_{0.06}\text{Sm}_{0.02}]_{\Sigma 0.50}\text{Mn}_{0.44})_{\Sigma 6}(\text{Mn}_{2.22}\text{Fe}_{0.78})_{\Sigma 3}(\text{Zr}_{2.71}\text{Ti}_{0.32})_{\Sigma 3.03}$ $(\text{W}_{0.78}\text{Nb}_{0.21})_{\Sigma 0.99}\text{Si}_{24.97}\text{O}_{73}(\text{CO}_3)(\text{OH},\text{Cl}_{0.75})_{\Sigma 2}$ $\text{Na}_{12}\text{Ce}_3\text{Ca}_6\text{Mn}_3\text{Zr}_3\text{WSi}_{25}\text{O}_{73}(\text{CO}_3)(\text{OH})_2$	[21]
Kentbrooksite	$(\text{Na}_{14.93}\text{REE}_{0.44}\text{Y}_{0.42}\text{K}_{0.30}\text{Sr}_{0.15})_{\Sigma 16.24}(\text{Ca}_{3.27}\text{Mn}_{1.78}\text{REE}_{0.62}\text{Na}_{0.33})_{\Sigma 6.00}$ $(\text{Mn}_{1.90}\text{Fe}_{0.72}\text{Al}_{0.13}\text{Mg}_{0.05})_{\Sigma 2.80}(\text{Nb}_{0.55}\text{Zr}_{0.12}\text{Ti}_{0.10})_{\Sigma 0.77}\text{Si}_{0.60}(\text{Zr}_{2.81}\text{Hf}_{0.06}\text{Ti}_{0.13})_{\Sigma 3}$ $[(\text{Si}_3\text{O}_9)_2(\text{Si}_9\text{O}_{27})_2\text{O}_2](\text{F}_{1.51}\text{Cl}_{0.27}\text{OH}_{0.22})_{\Sigma 2}\cdot 2.3\text{H}_2\text{O}$ $(\text{Na},\text{REE})_{15}(\text{Ca},\text{REE})_6\text{Mn}_3\text{Zr}_3\text{Nb}(\text{Si}_{25}\text{O}_{73})(\text{O},\text{OH},\text{H}_2\text{O})_3(\text{F},\text{Cl})_2$	[22]
Khomyakovite	$(\text{Na}_{12.26}\text{Ca}_{0.33}\text{K}_{0.38}\text{Sr}_{0.13}\text{REE}_{0.08})_{\Sigma 13.05}(\text{Sr}_{2.78}\text{Na}_{0.22})_{\Sigma 3}\text{Ca}_6(\text{Fe}_{2.05}\text{Mn}_{0.78}\text{Mg}_{0.03})_{\Sigma 2.86}$ $(\text{Zr}_{2.94}\text{Ti}_{0.05}\text{Hf}_{0.03})_{\Sigma 3.02}(\text{W}_{0.56}\text{Nb}_{0.34})_{\Sigma 0.90}(\text{Si}_{24.78}\text{Al}_{0.06})_{\Sigma 24.84}$ $\text{O}_{73}(\text{O},\text{OH},\text{H}_2\text{O})_{\Sigma 3.70}(\text{OH}_{1.36}\text{Cl}_{0.64})_{\Sigma 2}$ $\text{Na}_{12}\text{Sr}_3\text{Ca}_6\text{Fe}_3\text{Zr}_3\text{W}(\text{Si}_{25}\text{O}_{73})(\text{O},\text{OH},\text{H}_2\text{O})_3(\text{Cl},\text{OH})_2$	[23]
Labyrinthite	$\text{Na}_{33.19}\text{K}_{0.98}\text{Ca}_{11.68}\text{Sr}_{1.57}\text{Fe}_{2.19}\text{Mn}_{0.77}\text{Zr}_{5.95}\text{Ti}_{0.49}\text{Si}_{51.26}\text{Cl}_{3.04}\text{H}_{10.8}$ $(\text{Na},\text{K},\text{Sr})_{35}\text{Ca}_{12}\text{Fe}_3\text{Zr}_6\text{TiSi}_{51}\text{O}_{144}(\text{O},\text{OH},\text{H}_2\text{O})_9\text{Cl}_3$	[24]
Mangankhomakovite	$(\text{Na}_{11.51}\text{K}_{0.30}\text{Ca}_{0.25}\text{Sr}_{0.04}\text{REE}_{0.07})_{\Sigma 12.17}\text{Sr}_3\text{Ca}_6(\text{Mn}_{2.04}\text{Fe}_{1.23})_{\Sigma 3.27}(\text{Zr}_{2.91}\text{Hf}_{0.03}\text{Ti}_{0.01})_{\Sigma 2.95}$ $(\text{W}_{0.66}\text{Nb}_{0.41}\text{Ta}_{0.01})_{\Sigma 1.08}(\text{Si}_{24.60}\text{Al}_{0.01})_{\Sigma 24.61}\text{O}_{73}(\text{O},\text{OH},\text{H}_2\text{O})_{\Sigma 3.70}(\text{OH}_{1.19}\text{Cl}_{0.81})_{\Sigma 2}$ $\text{Na}_{12}\text{Sr}_3\text{Ca}_6\text{Mn}_3\text{Zr}_3\text{W}(\text{Si}_{25}\text{O}_{73})(\text{O},\text{OH},\text{H}_2\text{O})_3(\text{Cl},\text{OH})_2$	[23]
Manganoeudialyte	$\text{H}_{12.08}\text{Na}_{12.05}\text{Sr}_{0.90}\text{K}_{0.39}\text{La}_{0.03}\text{Ce}_{0.02}\text{Ca}_{5.93}(\text{Mn}_{1.54}\text{Fe}_{1.18})\text{Zr}_{3.03}\text{Nb}_{0.28}\text{Al}_{0.25}$ $\text{Hf}_{0.04}\text{Ti}_{0.18}\text{Si}_{25.20}\text{O}_{79.40}\text{Cl}_{0.87}\text{F}_{0.13}$ $\text{Na}_{14}\text{Ca}_6\text{Mn}_3\text{Zr}_3[\text{Si}_{26}\text{O}_{72}(\text{OH})_2](\text{H}_2\text{O},\text{Cl},\text{O},\text{OH})_6$	[25]
Mogovidite	$(\text{Na}_{9.87}\text{Ca}_{4.05}\text{K}_{0.24}\text{Ce}_{0.06}\text{La}_{0.03})_{\Sigma 14.25}\text{Ca}_{6.00}\text{Fe}^{3+}_{1.48}\text{Fe}^{2+}_{0.58}\text{Mn}_{0.30}\text{Zr}_{3.02}\text{Ti}_{0.09}(\text{Nb}_{0.40}\text{Si}_{0.71})$ $\text{Si}_{24}\text{O}_{72}(\text{OH})_{2.86}(\text{CO}_3)_{1.03}\text{Cl}_{0.46}\cdot 0.74\text{H}_2\text{O}$ $\text{Na}_9(\text{Ca},\text{Na})_{12}\text{Fe}_2\text{Zr}_3\text{Si}_{25}\text{O}_{72}(\text{CO}_3)(\text{OH})_4$	[18]
Odikhinchaita	$\text{H}_{8.22}\text{Na}_{9.97}\text{K}_{0.42}\text{Ca}_{7.59}\text{Sr}_{1.87}\text{Ce}_{0.08}\text{La}_{0.08}\text{Nd}_{0.03}\text{Mn}_{2.58}\text{Fe}_{0.35}\text{Mg}_{0.20}\text{Ti}_{0.03}\text{Zr}_{3.01}\text{Nb}_{1.05}$ $\text{Si}_{24.87}\text{Al}_{0.05}\text{Cl}_{0.65}\text{C}_{0.68}\text{O}_{81.71}$ $\text{Na}_9\text{Sr}_3[(\text{H}_2\text{O})_2\text{Na}]\text{Ca}_6\text{Mn}_3\text{Zr}_3\text{NbSi}(\text{Si}_{24}\text{O}_{73})(\text{OH})_3(\text{CO}_3)\cdot \text{H}_2\text{O}$	[26]
Oneillite	$(\text{Na}_{14.37}\text{REE}_{1.53}\text{K}_{0.20}\text{Sr}_{0.03})_{\Sigma 16.13}(\text{Ca}_{1.77}\text{REE}_{0.59}\text{Na}_{0.66})_{\Sigma 3.02}(\text{Mn}_{2.76}\text{Y}_{0.24})_{\Sigma 3.00}$ $(\text{Fe}_{1.43}\text{Mn}_{0.96}\text{Zr}_{0.25})_{\Sigma 2.64}(\text{Zr}_{2.93}\text{Nb}_{0.05}\text{Hf}_{0.03})_{\Sigma 3.01}(\text{Nb}_{0.85}\text{Ta}_{0.02})_{\Sigma 0.87}(\text{Si}_{24.77}\text{Al}_{0.12})_{\Sigma 24.89}$ $\text{O}_{73}(\text{O},\text{OH},\text{H}_2\text{O})_{\Sigma 2.00}(\text{OH}_{1.27}\text{Cl}_{0.73})_{\Sigma 2.00}$ $\text{Na}_{15}\text{Ca}_3\text{Mn}_3\text{Fe}_3\text{Zr}_3\text{Nb}(\text{Si}_{25}\text{O}_{73})(\text{O},\text{OH},\text{H}_2\text{O})_3(\text{OH},\text{Cl})_2$	[27]
Raslakite	$\text{Na}_{16.02}\text{K}_{0.32}\text{Ca}_{3.13}\text{Sr}_{0.21}\text{Mg}_{0.22}\text{Fe}_{2.17}\text{Mn}_{0.88}\text{Ce}_{0.16}\text{La}_{0.08}\text{Ti}_{0.14}\text{Zr}_{3.80}\text{Hf}_{0.06}\text{Nb}_{0.17}\text{Al}_{0.16}$ $\text{Si}_{25.40}\text{Cl}_{1.18}\text{H}_{4.66}\text{O}_{76.465}$ $\text{Na}_{15}\text{Ca}_3\text{Fe}_3(\text{Na},\text{Zr})_3\text{Zr}_3(\text{Si},\text{Nb})\text{Si}_{25}\text{O}_{73}(\text{OH},\text{H}_2\text{O})_3(\text{Cl},\text{OH})$	[19]
Rastsvetaevite	$\text{Na}_{27.10}(\text{K}_{7.93}\text{Ba}_{0.03})_{\Sigma 7.96}(\text{Ca}_{11.29}\text{Sr}_{0.74}\text{Ce}_{0.04})_{\Sigma 12.07}(\text{Fe}_{2.32}\text{Mn}_{0.42})_{\Sigma 2.74}(\text{Zr}_{5.69}\text{Ti}_{0.30}\text{Hf}_{0.04})_{\Sigma 6.03}$ $(\text{Si}_{51.53}\text{Al}_{0.20}\text{Nb}_{0.16}\text{Ta}_{0.01})_{\Sigma 51.90}\text{O}_{144}\text{O}_{2.14}(\text{OH})_{1.86}\text{Cl}_{2.29}\cdot 1.71\text{H}_2\text{O}$ $\text{Na}_{27}\text{K}_8\text{Ca}_{12}\text{Fe}_3\text{Zr}_6\text{Si}_{52}\text{O}_{144}(\text{OH},\text{O})_6\text{Cl}_2$	[28]
Sergevanite	$\text{H}_{14.46}\text{Na}_{13.64}\text{K}_{0.92}\text{Ca}_{4.22}\text{Ce}_{0.27}\text{La}_{0.17}\text{Nd}_{0.12}\text{Pr}_{0.06}\text{Sm}_{0.02}\text{Mn}_{1.81}\text{Fe}^{2+}_{0.58}\text{Ti}_{0.46}\text{Zr}_{2.67}$ $\text{Hf}_{0.04}\text{Nb}_{0.38}\text{Si}_{25.5}\text{S}_{0.30}\text{Cl}_{0.20}\text{O}_{81}$ $\text{Na}_{15}(\text{Ca}_3\text{Mn}_3)(\text{Na}_2\text{Fe})\text{Zr}_3\text{Si}_{26}\text{O}_{72}(\text{OH})_3\cdot \text{H}_2\text{O}$	[29]
Siudaite	$[\text{Na}_{7.57}(\text{H}_2\text{O})_{1.43}]_{\Sigma 9}(\text{Mn}_{1.11}\text{Na}_{0.88}\text{Ce}_{0.31}\text{La}_{0.20}\text{Nd}_{0.05}\text{Pr}_{0.04}\text{K}_{0.41})_{\Sigma 3}(\text{H}_2\text{O})_{1.8}(\text{Ca}_{5.46}\text{Mn}_{0.54})_{\Sigma 6}$ $(\text{Fe}^{3+}_{1.76}\text{Mn}^{2+}_{1.19})_{\Sigma 2.95}\text{Nb}_{0.65}(\text{Ti}_{0.20}\text{Si}_{0.50})_{\Sigma 0.71}(\text{Zr}_{2.95}\text{Hf}_{0.04}\text{Ti}_{0.01})_{\Sigma 3}$ $\text{Si}_{24.00}\text{Cl}_{0.47}\text{O}_{70}(\text{OH})_2\text{Cl}_{0.47}\cdot 1.82\text{H}_2\text{O}$ $\text{Na}_8(\text{Mn}_2\text{Na})\text{Ca}_6\text{Fe}^{3+}_3\text{Zr}_3\text{NbSi}_{25}\text{O}_{74}(\text{OH})_2\text{Cl}\cdot 5\text{H}_2\text{O}$	[30]
Taseqite	$(\text{Na}_{8.81}\text{Sr}_{4.78}\text{K}_{0.17}\text{Ce}_{0.02})_{\Sigma 13.78}(\text{Ca}_{5.17}\text{Mn}_{0.59}\text{Y}_{0.09})_{\Sigma 5.85}(\text{Fe}_{1.93}\text{Mn}_{0.92})_{\Sigma 2.85}(\text{Zr}_{2.84}\text{Nb}_{0.11}\text{Hf}_{0.05})_{\Sigma 3.00}$ $(\text{Nb}_{1.06}\text{Ta}_{0.04}\text{Sn}_{0.03})_{\Sigma 1.13}\text{Si}_{24.55}\text{O}_{73}(\text{O}_{1.65}\text{OH}_{0.75}(\text{H}_2\text{O})_{0.74})_{\Sigma 3.14}(\text{Cl}_{1.91}\text{OH}_{0.09})_{\Sigma 2.00}$ $\text{Na}_{12}\text{Sr}_3\text{Ca}_6\text{Fe}_3\text{Zr}_3\text{NbSi}_{25}\text{O}_{73}(\text{O},\text{OH},\text{H}_2\text{O})_3\text{Cl}_2$	[31]

Table 1. Cont.

Mineral	Empirical Formula */IMA Formula	Ref.
Voronkovite	(Na _{13.96} Sr _{0.54} K _{0.19}) _{Σ14.69} (Na _{1.64} Ca _{0.92} Ce _{0.26} La _{0.18}) _{Σ3.00} (Mn _{2.06} Ca _{0.81} Nd _{0.13}) _{Σ3.00} (Fe _{1.54} Zr _{0.60} Na _{0.48} Nb _{0.21} Ti _{0.13} Hf _{0.04}) _{Σ3.00} Zr _{3.00} (Si _{1.91} Al _{0.09}) _{Σ2.00} (Si ₂₄ O ₇₂)[(OH) _{2.98} O _{1.02}] _{Σ4} (Cl _{0.39} F _{0.35}) _{Σ0.74} ·1.23H ₂ O Na ₁₅ (Na,Ca,Ce) ₃ (Mn,Ca) ₃ Fe ₃ Zr ₃ Si ₂₆ O ₇₂ (OH,O) ₄ Cl·H ₂ O	[32]
Zirsilite-(Ce)	(Na _{9.01} Ca _{0.82} K _{0.32}) _{Σ10.15} [(Ce _{0.76} La _{0.47} Nd _{0.16} Pr _{0.06}) _{Σ1.45} Na _{1.12} Sr _{0.43}] _{Σ3} (Ca _{5.36} Mn _{0.50} Y _{0.14}) _{Σ6} (Mn _{2.13} Fe _{0.87}) _{Σ3} (Zr _{2.80} Ti _{0.18}) _{Σ2.98} Nb _{0.93} Si ₂₅ H _{5.54} (CO ₃) _{0.43} Cl _{0.30} (Na, \square) ₁₂ (Ce,Na) ₃ Ca ₆ Mn ₃ Zr ₃ NbSi ₂₅ O ₇₃ (OH) ₃ (CO ₃)·H ₂ O	[10]

* as it was published in the paper with the description of the new mineral species.

Table 2. Site occupancies of the IMA-approved members of the eudialyte group.

Mineral	Space Group	N(1)	N(2)	N(3)	N(4)	N(5)	Z	M(1a)	M(1b)	M(2)	M(3)	M(4)	X(1)	X(2)
Alluaivite	R̄3m	Na	Na	Na	Na	Na	Ti	Ca Ca		□, Na Na	Si	Si	H ₂ O	Cl
Andrianovite	R3m	Na	Na	Na	K	Na	Zr	Ca		Mn	Nb	Si	H ₂ O	CO ₃
Aqualite	R3	H ₃ O	Na	H ₃ O	H ₃ O	□, OH	Zr	Ca	Ca	□, Na	Si	Si	Cl, SO ₄	Cl
Carbokentbrooksite	R3m	Na	Na	Na	Na	Na	Zr	Ca		Mn	Nb	Si	CO ₃	H ₂ O
Davinciite	R3m	Na	Na	K	Na	Na	Zr	Ca		Fe ²⁺	Si	Si	H ₂ O	Cl
Dualite	R3m	Na	Na	Na	Na	Na	Zr	Ca		Na	Si	Si	H ₂ O	Cl
Eudialyte	R3m	Na	Na	Na	Na	Na	Zr	Ca		Fe ²⁺	Si	Si	Cl	H ₂ O
Feklichevite	R3m	Na	Na	Ca	Na	Na	Zr	Ca		Fe ³⁺	Nb	Si	H ₂ O	Cl
Fengchengite	R̄3m	Na	Na	□	Na	Na	Zr	Ca		Fe ³⁺	Si	Si	Cl	OH
Ferrokentbrooksite	R3m	Na	Na	Na	Na	Na	Zr	Ca		Fe ²⁺	Nb	Si	Cl	F
Georgbarsanovite	R3m	Na	Na	Na	Mn	Na	Zr	Ca		Fe ²⁺	Nb	Si	Cl	H ₂ O
Golyshevite	R3m	Na	Na	Na	Ca	□, Na	Zr	Ca		Fe ³⁺	Si	Nb	CO ₃	H ₂ O
Ikranite	R3m	H ₃ O	Na	Na	Na	□, OH	Zr	Ca		Fe ³⁺	□	□	H ₂ O	H ₂ O
Ilyukhinite	R3m	H ₃ O	H ₃ O	H ₃ O	Na	H ₃ O	Zr	Ca		Mn	Si	Si	H ₂ O	H ₂ O
Johnsenite-(Ce)	R3m	Na	Na	Na	REE	Na	Zr	Ca		Mn	W	Si	CO ₃	H ₂ O
Kentbrooksite	R3m	Na	Na	Na	Na	Na	Zr	Ca		Mn	Nb	Si	F	F
Khomyakovite	R3m	Na	Na	Na	Sr	Na	Zr	Ca		Fe	W	Si	OH	Cl
Labyrinthite	R3	Na	Na	Na	Na	Na	Zr	Ca	Ca	Na	Ti	Si	Cl, F	Cl
		Na	Na	Na	Na	Na	Zr	Ca	Ca	Fe	Si	Si	H ₂ O	Cl
Mangankhomyakovite	R3m	Na	Na	Na	Sr	Na	Zr	Ca		Mn	W	Si	OH	Cl
Manganoeudialyte	R3m	Na	Na	Na	Na	Na	Zr	Ca		Mn	Si	Si	H ₂ O	H ₂ O
Mogovidite	R3m	Na	Na	Ca	Ca	Na	Zr	Ca		Fe ³⁺	□, Nb	Si	CO ₃	H ₂ O
Odikhinchaite	R3m	Na	Na	Sr	Na	H ₂ O	Zr	Ca		Mn	Nb	Si	CO ₃	H ₂ O
Oneillite	R3	Na	Na	Na	Na	Na	Zr	Mn	Ca	Fe	Nb	Si	H ₂ O	H ₂ O
Raslakite	R3	Na	Na	Na	Na	Na	Zr	Ca	Fe	Na	Si	Si	H ₂ O	Cl
Rastsvetaevite	R3m	Na	Na	Na	Na	Na	Zr	Ca		K	Si	Si	H ₂ O	Cl
		Na	Na	K	Na	Na	Zr	Ca		Fe	Si	Si	Cl	Cl
Sergevanite	R3	Na	Na	Na	Na	H ₂ O	Zr	Ca	Mn	Na	Si	Si	H ₂ O	Cl
Siudaite	R3m	Na	Na	Na	Mn	H ₂ O	Zr	Ca		Fe ³⁺	Nb	Si	Cl	H ₂ O
Taseqite	R3m	Na	Na	Na	Sr	Na	Zr	Ca		Fe ²⁺	Nb	Si	Cl	Cl
Voronkovite	R3	Na	Na	Na	Na	Na	Zr	Na	Mn	Fe	Si	Si	H ₂ O	H ₂ O
Zirsilite-(Ce)	R3m	Na	Na	Na	Ce	Na	Zr	Ca		Mn	Nb	Si	CO ₃	H ₂ O

RREGMs are widely used in petrological studies. Together with other Na-Ca-HFSE minerals (i.e., rinkite, wöhlerite, aenigmatite, astrophyllite, catapleiite, etc.) they are considered as mineralogical markers of agpaitic rocks [33] which attract economic interest as the most promising sources for future high-field-strength elements (HFSE) and rare earth elements (REE) supply [34,35]. Moreover, the highly variable composition of EGMs may be used to study the compositional and/or physical-chemical changes during the evolution of magmatic and hydrothermal systems [36–39].

In this case, because of the great economic, petrological, and mineralogical significance of the EGMs, an express diagnostic based on microprobe data is especially important. However, the large number of framework and extraframework sites in the crystal structure (which can be partial or completely vacant), the different types of cation distributions, and the presence and predominance of the same element at one or more sites make it difficult to give a name to a sample of EGMs based only on the chemical composition (without additional single-crystal X-ray diffraction analysis, IR- and Mössbauer spectroscopy). Originally, a possible way to determine the mineral species based on the empirical formula was proposed by Johnsen and Grice [1]. Pfaff with coauthors [40] presented an extended and improved scheme for site assignment using IMA-approved end-members also based on microprobe analyses (however, the different valence states of Fe and Mn and undetermined H₂O-contents were ignored in these studies).

Later, Rastsvetaeva and Chukanov [3] proposed a hierarchical crystal chemical scheme for the classification of EGMs (without formal approval by the CNMNC IMA) which contains the following features steps:

1. The value of *c* parameter (~30 Å or ~60 Å for “12-layer” and “24-layer” members, respectively);
2. Cation ordering in octahedral six-membered [M(1)₆O₂₄] rings, i.e., ring of six calcium atoms vs. ring with alternating atoms of different elements (Ca + Mn, Ca + Fe, Mn + Na);
3. What elements (or vacancies) prevail in centers of [Si₉O₂₇] rings: Si, Nb, Ti, W, Mn;
4. What elements prevail M(2)O_n polyhedra;
5. What elements prevail N(3) and N(4) polyhedra;
6. The water content [Na > (H₂O + H₃O⁺) or Na < (H₂O + H₃O⁺)].

Based on this classification scheme and taking into account the data on the site occupancy in the crystal structures of different EGMs (Table 2), we propose a new algorithm that makes it possible to determine minerals based on chemical data only without a direct site assignment procedure. Our diagnostic scheme consists of the following steps:

- (1) Zr or Ti in Z site;
- (2) Division according to the assignment of the M(1) site;
- (3) Division according to the occupation of M(3) and M(4) sites;
- (4) Division according to population of the M(2), N(3), N(4) sites.

2. Methods

The diagnostic scheme has been developed in accordance with the principles and rules of the Commission on New Minerals and Mineral Names of the International Mineralogical Association. The list of eudialyte-group minerals was taken from IMA list of minerals 2021 (<http://cmmnc.main.jp/imalist.htm> accessed on 20 November 2021).

3. Diagnostic Scheme of EGMs

The proposed diagnostic scheme is based on the values of the formula coefficients of the elements, which must be normalized on Si+Al+Ti+Zr+Hf+Nb+Ta+W = 29 [1]. After that, the *apfu* values of species-forming elements are considered step-by-step.

3.1. Framework Cations: Zirconium or Titanium in Z Site (Step 1)

In all “12-layer” minerals, as well as “24-layer” rastsvetaevite and labyrinthite, ZO_6 octahedra are occupied by zirconium and there are no other structural sites in which zirconium dominates. In the crystal structure of “24-layer” dualite, a half of the zirconium is replaced by titanium, while in the “24-layer” alluaivite, titanium fully occupies the ZO_6 octahedra. To establish the corresponding values of *apfu* for Zr and Ti at Z site, the following case should be considered:

- (1) Zirconium fully occupies Z site;
- (2) Titanium fully occupies Z site;
- (3) Half of zirconium is replaced by titanium.

Let us assume that $Z = Zr_3Ti_3$ in dualite ($=Zr_{1.5}Ti_{1.5}$ in comparison with “12-layer”), $Z = Ti_6$ in alluaivite ($=Ti_3$ in comparison with “12-layer”), and $Z = Zr_3$ in other minerals (as well as in “24-layer” rastsvetaevite and labyrinthite). In accordance with IMA–CNMNC dominant–constituent rule [41], the content of Zr in Z site should be: is $0.75 < Zr < 2.25 \text{ apfu}$ in dualite; $Zr < 0.75 \text{ apfu}$ in alluaivite; $Zr > 2.25 \text{ apfu}$ in other minerals. Thus, at the first step, all members of the eudialyte group are divided into ***zirconium-titanium eudialytes*** (represented only by “24-layer” dualite and alluaivite), and ***zirconium eudialytes*** (all “12-layer” minerals and “24-layer” rastsvetaevite and labyrinthite).

3.2. Framework Cations: Calcium at the M(1) Site (Step 2)

Calcium is normally the predominant element at M(1) site with Mn and REE as the common substituents and in most “12-layer” members of the eudialyte group, the M(1) site is occupied by Ca. In low-calcium members of the EGM (oneillite, raslakite, sergevanite, voronkovite, and their varieties) the $Ca/(Ca + Mn + REE)$ ratio in M(1) site decreases and the $M(1)O_6$ octahedron ($\langle M(1)-O \rangle \sim 2.35(2) \text{ \AA}$) becomes more distorted. In this case, the M(1) site splits into two symmetrically nonequivalent M(1a) and M(1b) sites at the centers of small $M(1a)O_6$ octahedra ($\langle M(1a)-O \rangle \sim 2.227 \text{ \AA}$) occupied predominantly by Mn^{2+} (oneillite and sergevanite) or Fe^{2+} (raslakite) and a relatively large $M(1b)O_6$ ($\langle M(1b)-O \rangle \sim 2.431 \text{ \AA}$) octahedra occupied by Ca¹. If Ca atoms predominate over other cations at M(1) site, the condition $Ca > 4.5 \text{ apfu}$ must be satisfied. This value is the boundary for dividing ***zirconium eudialytes*** (Figure 2) into ***Ca-rich zirconium eudialytes*** ($Ca > 4.5 \text{ apfu}$) and ***Ca-poor zirconium eudialytes*** ($Ca \leq 4.5 \text{ apfu}$).

It should also be noted that in the holotype samples of kentbrooksite and ikranite, the M(1) site is not fully occupied by calcium, but the corresponding split of this site (due to the symmetry reducing like in oneillite, raslakite, and voronkovite) has not been observed. In holotype kentbrooksite, the composition of the M(1) site is $(Ca_{0.545}Mn_{0.297}REE_{0.103}Na_{0.05})$ or $(Ca_{3.27}Mn_{1.78}REE_{0.62}Na_{0.33})_{\Sigma 6}$ for the whole $[M(1)_6O_{24}]$ ring). The IMA-formula of kentbrooksite is approved without specification of the amount of calcium, therefore, kentbrooksite should be attributed to the ***Ca-rich zirconium eudialytes***. The ikranite holotype sample also contains a low amount of calcium without split of the M(1) site due to symmetry reducing. Ikranite will be attributed to ***Ca-poor zirconium eudialytes***.

3.3. Framework Cations: Occupation of the M(3) and M(4) Sites (Step 3)

The following variants of filling the M(3) and M(4) sites are possible: two additional $SiO_3\emptyset$ -tetrahedra ($T + T$), a $SiO_3\emptyset$ -tetrahedron and $MO_3\emptyset_3$ -octahedron ($T + M$), a $SiO_3\emptyset$ -tetrahedron and a vacancy ($T + \square$), and two vacancies ($\square + \square$). In the case of $M(3) + M(4) = T + M$, M is either niobium or tungsten (in Ca-rich zirconium eudialytes) or only niobium (in Ca-poor zirconium eudialytes).

For $T + T$ members, the following conditions are required:

1. $Si > 25.5 \text{ apfu} \{[Si_{24}O_{72}] + {}^{M(3)}Si\varphi_4 + \frac{1}{2}{}^{M(4)}Si\varphi_4\};$
2. $Nb \leq 0.5 \text{ apfu}$
3. $W \leq 0.5 \text{ apfu}$

For $T + M$ members, the following condition is required: $24.5 < Si \leq 25.5 \text{ apfu}$.

Minerals $T + M$ with a predominance of niobium must additionally meet the condition $Nb > 0.5 \geq W$. Tungsten is the species-forming element if the following conditions are met: $24.5 < Si \leq 25.5$; $W > 0.5 \geq Nb$.

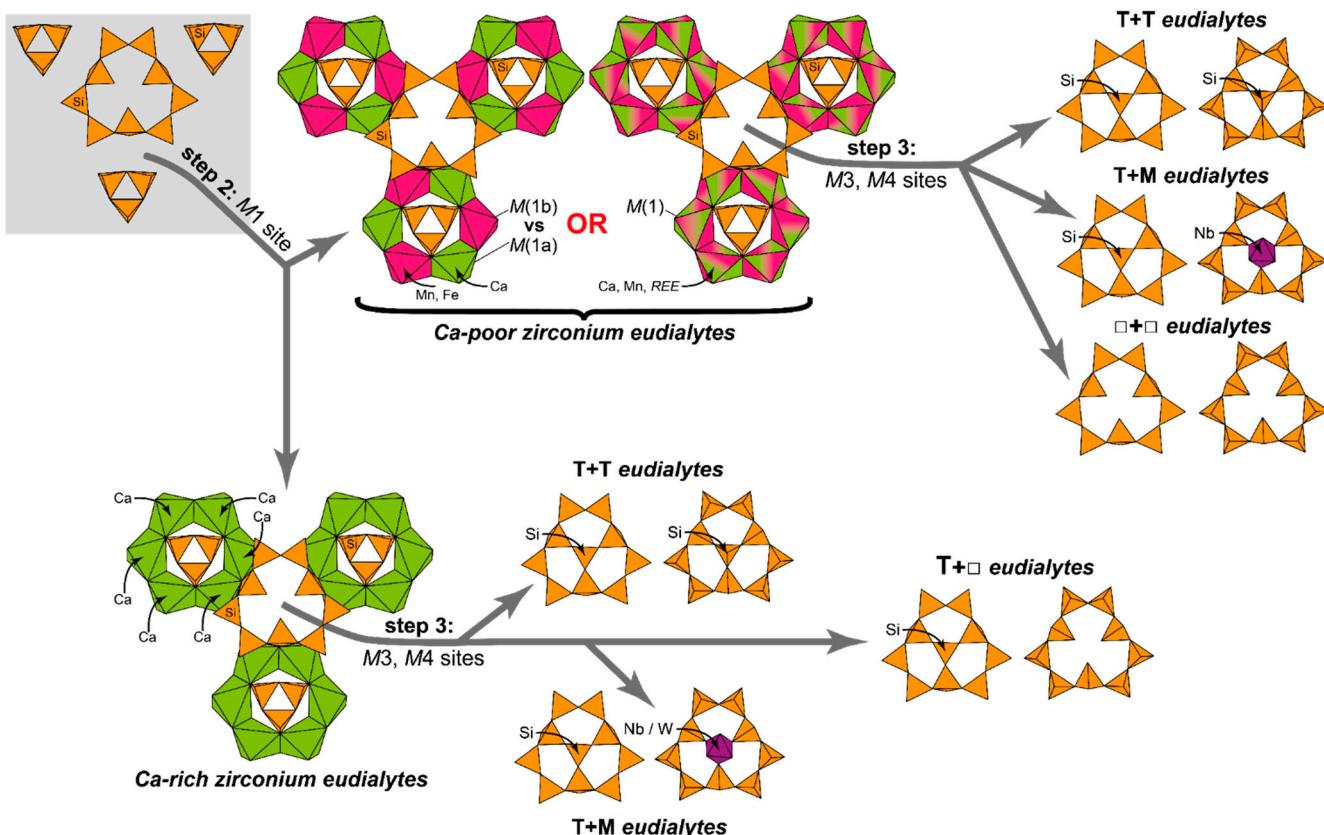


Figure 2. Schematic sketch of the second and third steps of EGMs diagnostic. Based on Rastsvetaeva and Chukanov (2012) [3].

It should be noted that the normalization $Si + Al + Ti + Zr + Hf + Nb + Ta + W = 29$ implies complete filling of the positions $Z_3M(3)M(4)Si_{24}$ [1]. However, in the case of the presence of vacancies in either the $M(3)$ or the $M(4)$ sites, such a calculation may lead to unreliable results.

The presence of vacancies can only be accurately established using additional methods, for example, spectroscopic ones. In the IR spectra of EGMs with additional SiO_4 tetrahedra located at the centers of nine-membered rings, there are bands in the range $905\text{--}940\text{ cm}^{-1}$. Bands in the range $676\text{--}689\text{ cm}^{-1}$ indicate additional NbO_6 and WO_6 octahedra at the centers of the nine-membered rings. Figure 3 shows for comparison the IR spectra of holotype samples of manganoeudialyte, oneillite, mogovidite, and ikranite. Obviously, IR spectroscopy data increase the accuracy of diagnostics of EGMs.

Let us consider different options for calculating the formula for holotype samples of mogovidite (vacancy in $M(3)$ site) and ikranite (vacancies in $M(3)$ and $M(4)$ sites) (Table 3).

As can be seen from Table 3, the choice of the basis for calculating the formula significantly affects the values of the formula coefficients for minerals with a predominance of vacancies in the $M(3)$ and/or $M(4)$ sites. The value of $Si\text{ pfu}$ increases most significantly, since its share in the basis for calculating of the EGM formula is the highest (at least 24 $apfu$). However, neither in the case of mogovidite, nor in the case of ikranite, does the $Si\text{ pfu}$ exceed 25.5. Normalization on $Si + Al + Ti + Zr + Hf + Nb + Ta + W = 29$ for mogovidite and ikranite shows the Si content as in $T + M$ eudialytes, but at the same time a low niobium content. This is because the $M(3)$ site in the mogovidite and the $M(3)$ and $M(4)$ sites in the ikranite are partially occupied. So, in the crystal-chemical formula of mogovidite,

the populations of the $M(3)$ and $M(4)$ sites are as follows: $M^3[\square_{0.58}Nb_{0.21}Si_{0.21}]M^4[Si_{0.5}Nb_{0.2}Ti_{0.1}\square_{0.2}]$ [18], and in ikranite $M^3[\square_{0.56}Si_{0.21}Zr_{0.08}Nb_{0.03}Ti_{0.03}]M^4[\square_{0.54}Zr_{0.32}Nb_{0.07}Ti_{0.07}]$ [19]. Therefore, the presence of vacancies in the $M(3)$ and $M(4)$ sites is indirectly indicated by the values $24.5 < Si \leq 25.5$ and $Nb \leq 0.5$; $W \leq 0.5$. Since mogovidite and ikranite differ significantly in calcium content, their separation in the proposed diagnostic scheme does not cause difficulties.

So, based on the occupancies of the $M(3)$ and $M(4)$ sites, the *Ca-rich zirconium eudialytes* are divided into $T+T$, $T+Nb$, $T+W$, $T+\square$ *eudialytes*, while the *Ca-poor zirconium eudialytes* are divided into $T+T$, $T+Nb$, $\square+\square$ *eudialytes* (Figure 2).

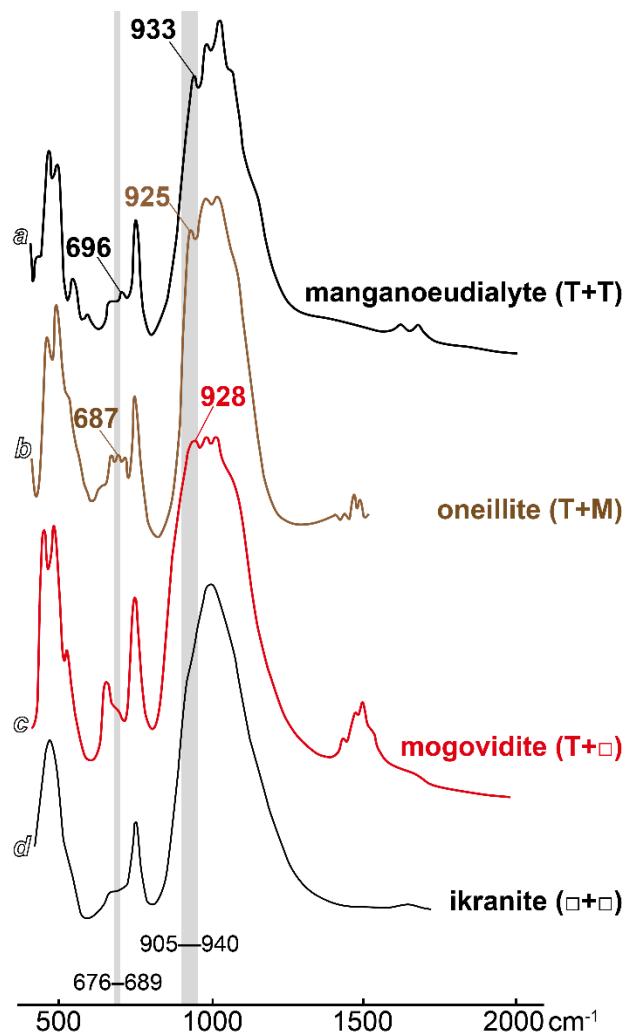


Figure 3. IR spectra of holotype samples of manganoeudialyte [25] (a), oneillite [27] (b), mogovidite [18] (c), and ikranite [19] (d). The spectra of manganoeudialite, oneillite, and mogovidite contain bands corresponding to additional SiO_4 tetrahedra located at the centers of nine-membered rings ($933, 925, 928\text{ cm}^{-1}$, respectively).

3.4. Ca-Rich Zirconium Eudialytes: Occupation of the $M(2)$ Site (Step 4)

Before the consideration of the assignment of the $M(2)$ site by manganese and/or iron, one should take into account that part of the manganese can be included in the $M(1)_6O_{24}$ ring. For minerals which contain $4.5\text{ apfu} \leq ^{\text{Total}}\text{Ca} < 6\text{ apfu}$, the lack of cations in $M(1) = 6\text{ apfu} - ^{\text{Total}}\text{Ca}$ is first calculated. The lack of cations is compensated by manganese, and if it is not sufficient, then REE, then Na, and Fe [1]. The remainder of manganese $M^{(2)}\text{Mn} = ^{\text{Total}}\text{Mn} - M^{(1)}\text{Mn}$ belongs to $M(2)$ site. Accordingly, the remainder of the REE is

$N_{REE} = \text{Total}_{REE} - M^{(1)}_{REE}$. For other elements: $M^{(2)}_{Fe} = \text{Total}_{Fe} - M^{(1)}_{Fe}$ [where $M^{(2)}_{Fe} = M^{(2)}_{(Fe^{2+} + Fe^{3+})}$], $N_{Na} = \text{Total}_{Na} - M^{(1)}_{Na}$.

Table 3. Calculation of formula coefficients for holotype samples of ikranite and mogovidite.

Cation/Anion	Ikranite *		Mogovidite **	
	$Si = 24^{19}$	$Si + Al + Ti + Zr + Hf + Nb + Ta + W = 29$	$Si = 24.71^{18}$	$Si + Al + Ti + Zr + Hf + Nb + Ta + W = 29$
Nb	0.06	0.06	0.40	0.42
Si	24	25.28	24.71	25.39
Ti	0.14	0.14	0.09	0.09
Zr	3.33	3.51	3.02	3.10
Hf	0.04	0.04	-	-
Fe^{3+}	1.77	1.87	1.48	1.52
La	0.11	0.12	0.03	0.03
Ce	0.27	0.29	0.05	0.05
Nd	0.03	0.04	-	-
Fe^{2+}	0.16	0.16	0.57	0.59
Mn	1.41	1.49	0.30	0.31
Ca	3.31	3.48	10.05	10.33
Sr	0.46	0.48	-	-
Na	7.56	7.97	9.87	10.14
K	0.27	0.29	0.24	0.25
Cl	0.74	0.78	0.46	0.47
F	0.15	0.16	-	-

* Ikranite chemical composition [19]: SiO_2 48.91, TiO_2 0.37, Fe_2O_3 4.80, FeO 0.38, MnO 3.40, CaO 6.29, Na_2O 7.95, K_2O 0.44, Cl 0.89, F 0.10, H_2O 7.70, SrO 1.61, ZrO_2 13.94, Nb_2O_5 0.28, La_2O_3 0.62, Ce_2O_3 1.53, Nd_2O_3 0.19, HfO_2 0.28, sum 99.68. ** Mogovidite chemical composition [18]: SiO_2 47.49, TiO_2 0.23, Fe_2O_3 3.78, FeO 1.32, MnO 0.68, CaO 18.03, Na_2O 9.78, K_2O 0.36, Cl 0.52, ZrO_2 11.90, Nb_2O_5 1.72, La_2O_3 0.15, Ce_2O_3 0.28, H_2O 1.25, CO_2 1.42 sum 98.91.

If manganese or iron dominate in the crystal structure of eudialyte only in the M2 position, then the condition $4.5 \geq M^{(2)}_{Mn} + M^{(2)}_{Fe} > 1.5$ must be satisfied; if the M2 position is vacant, then the condition $M^{(2)}_{Mn} + M^{(2)}_{Fe} \leq 1.5$ must be satisfied. Additional conditions, such as $M^{(2)}_{Fe} > M^{(2)}_{Mn}$ or $M^{(2)}_{Mn} > M^{(2)}_{Fe}$, as well as $Fe^{3+} > Fe^{2+}$ or $Fe^{2+} > Fe^{3+}$, allow the separation of Mn-dominant and Fe-dominant end terms, as well as eudialytes with a predominance of ferrous or ferric iron.

Thus, $T + T$ eudialytes include the *eudialyte subgroup* ($4.5 \geq M^{(2)}_{Mn} + M^{(2)}_{Fe} > 1.5$; $M^{(2)}_{Fe} > M^{(2)}_{Mn}$; $Fe^{2+} > Fe^{3+}$), *fengchengite subgroup* ($4.5 \geq M^{(2)}_{Mn} + M^{(2)}_{Fe} > 1.5$; $M^{(2)}_{Fe} > M^{(2)}_{Mn}$; $Fe^{3+} > Fe^{2+}$), *manganoeudialyte subgroup* ($4.5 \geq M^{(2)}_{Mn} + M^{(2)}_{Fe} > 1.5$; $M^{(2)}_{Mn} > M^{(2)}_{Fe}$), and *aqualite subgroup* ($M^{(2)}_{Mn} + M^{(2)}_{Fe} \leq 1.5$). Among the $T + M$ eudialytes in the case of $4.5 \geq M^{(2)}_{Mn} + M^{(2)}_{Fe} > 1.5$; $M^{(2)}_{Fe} > M^{(2)}_{Mn}$, *ferrokentbrooksite* and *khomyakovite subgroups* are distinguished, and in the case of $4.5 \geq M^{(2)}_{Mn} + M^{(2)}_{Fe} > 1.5$; $M^{(2)}_{Mn} > M^{(2)}_{Fe}$ are *kentbrooksite* and *mangankhomyakovite subgroups*. Mogovidite is representative of $T + \square$ eudialytes with $4.5 \geq M^{(2)}_{Mn} + M^{(2)}_{Fe} > 1.5$, $M^{(2)}_{Fe} > M^{(2)}_{Mn}$, and its potential manganese analog will have the ratio $M^{(2)}_{Mn} > M^{(2)}_{Fe}$.

In siudaite and georgbarsanovite, $M^{(2)}_{Mn} + M^{(2)}_{Fe} > 4.5$, which corresponds to the complete filling of the M(2) site and the predominance of one of these elements in the N(4) site (*siudaite* and *georgbarsanovite subgroups*). In minerals of the siudaite subgroup, iron is trivalent, and in minerals of the georgbarsanovite subgroup, it is bivalent. It is important to note that in our scheme, the values of $M^{(2)}_{Fe}$ or $M^{(2)}_{Mn}$ are used only to assess

the deficiency or excess of cations in the considered sites. Therefore, the value of $M(2)\text{Mn} + M(2)\text{Fe} > 4.5$ with a maximum content of cations in $M(2)$ equal to three, indicates only that $M(2)$ is completely populated and there is an excess (1.5 *apfu* and more) content of the sum Mn and Fe.

EGMs can be enriched by calcium ($\text{Ca} > 6 \text{ apfu}$) and in addition to $M(1)$ site the excess of Ca can occupy the extraframework $N(3)$ and $N(4)$ sites. The excess calcium (${}^N\text{Ca} = {}^{\text{Total}}\text{Ca} - 6 \text{ apfu}$) will then be considered together with the elements assigned the N sites: Sr, REE, and K. In feklichevite, golyshevite, and mogovidite, ${}^N\text{Ca} > 1.5 \text{ apfu}$, since calcium in these minerals not only fills the six-membered $[M(1)_6\text{O}_4]$ rings, but also predominates in $N(3)$ site (feklichevite, golyshevite) or $N(3)$ and $N(4)$ sites (mogovidite).

Schematically, variants for filling positions in the structure of EGMs with iron and/or manganese are shown in Figure 4.

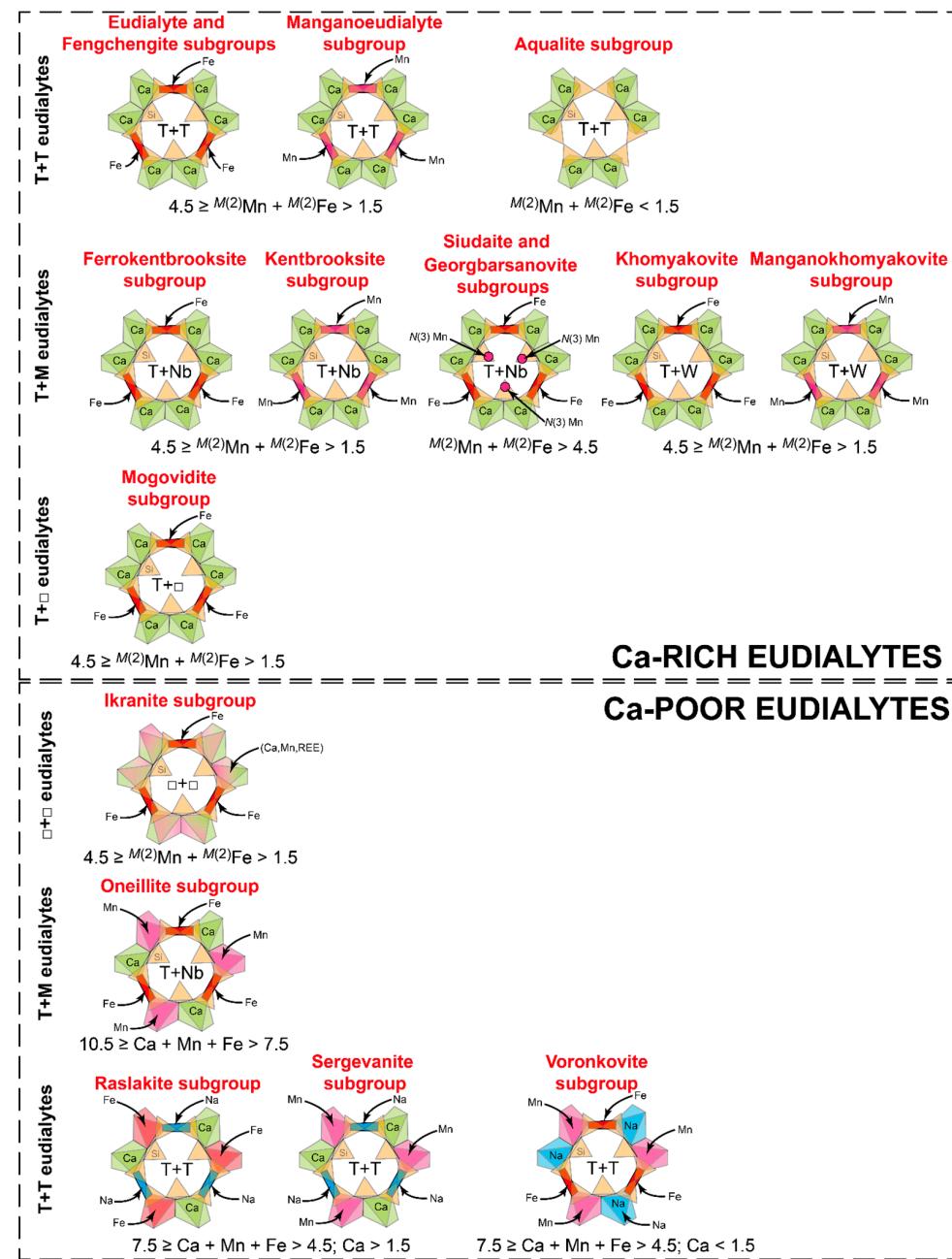


Figure 4. Options for filling $M(1)$, $M(2)$ and $N(3)$ sites with iron and manganese.

3.5. Ca-Poor Eudialytes: Occupation of the M(1) and M(2) Sites (Step 4)

Eudialytes $\square + \square$ are not divided into subgroups, since they contain only ikranite, for which $4.5 \geq {}^{M(2)}\text{Mn} + {}^{M(2)}\text{Fe} > 1.5$ and ${}^{M(2)}\text{Fe} > {}^{M(2)}\text{Mn}$.

For $T + M$ and $T + T$ Ca-poor eudialytes, the sequence of calculations is as follows:

1. An estimate of the sum $\text{Ca} + \text{Mn} + \text{Fe}$, i.e., the total content of cations in the $M(1a)$, $M(1b)$, and $M(2)$ sites. If only Ca, Mn, or Fe prevail in the listed sites, then the sum will be from 7.5 to 10.5 *apfu*. If the listed positions contain other species-forming elements (for example, sodium in the $M(2)$ site in raslakite and sergevanite), then the $\text{Ca} + \text{Mn} + \text{Fe}$ sum will be in the range from 7.5 to 4.5 *apfu*.
2. Assessment of the calcium content. If calcium dominates in one of the positions, for example, $M(1a)$, then the condition $\text{Ca} > 1.5 \text{ apfu}$ must be satisfied. In voronkovite, calcium is not a species-forming element and in this mineral $\text{Ca} < 1.5 \text{ apfu}$.
3. If $\text{Ca} > 1.5 \text{ apfu}$, then the following is an estimate of the content of manganese and iron in position $M(1)$. First, the difference between calcium content and 6 is compensated by manganese ${}^{M(1)}\text{Mn} = 6 - {}^{\text{Total}}\text{Ca}$, and then, if manganese is insufficient, by iron ${}^{M(1)}\text{Fe} = 6 - ({}^{M(1)}\text{Mn} + {}^{\text{Total}}\text{Ca})$. The remainder of manganese and iron is assigned to position $M(2)$: ${}^{M(2)}\text{Mn} = {}^{\text{Total}}\text{Mn} - {}^{M(1)}\text{Mn}$ and ${}^{M(2)}\text{Fe} = {}^{\text{Total}}\text{Fe} - {}^{M(1)}\text{Fe}$.

$T + M$ eudialytes include the *oneillite subgroup*, the only representative of which, oneillite, contains $10.5 \geq \text{Ca} + \text{Mn} + \text{Fe} > 7.5$; $\text{Ca} > 1.5$; ${}^{M(1)}\text{Mn} > {}^{M(1)}\text{Fe}$; ${}^{M(2)}\text{Fe} > {}^{M(2)}\text{Mn}$ (manganese and iron fill the $M1a$ and $M2$ positions). The $T + T$ eudialytes include the *sergevanite subgroup* ($7.5 \geq \text{Ca} + \text{Mn} + \text{Fe} > 4.5$; $\text{Ca} > 1.5$; ${}^{M(1)}\text{Mn} > {}^{M(1)}\text{Fe}$; ${}^{M(2)}\text{Fe} > {}^{M(2)}\text{Mn}$), the *raslakite subgroup* ($7.5 \geq \text{Ca} + \text{Mn} + \text{Fe} > 4.5$; $\text{Ca} > 1.5$; ${}^{M(1)}\text{Fe} > {}^{M(1)}\text{Mn}$; ${}^{M(2)}\text{Fe} > {}^{M(2)}\text{Mn}$) and the *voronkovite subgroup* ($7.5 \geq \text{Ca} + \text{Mn} + \text{Fe} > 4.5$; $\text{Ca} < 1.5$; ${}^{M(1)}\text{Mn} > {}^{M(1)}\text{Fe}$).

3.6. Extraframework Cations (N Sites)

Further separation of EGMs should be performed in accordance with the filling of N sites, namely, according to values of ${}^N\text{Na}$, ${}^N\text{Ca}$, K, Sr, ${}^N\text{REE}$ *apfu*. If potassium predominates in one of the N sites (for example, andrianovite), the conditions ${}^N\text{Na} > 10.5$; $K > 1.5$; ${}^N\text{Ca} < 1.5$; ${}^N\text{REE} < 1.5$; $Sr < 1.5$ must be satisfied simultaneously. If strontium predominates, as in odikhinchaite, then the conditions ${}^N\text{Na} > 7.5$; $K < 1.5$; ${}^N\text{Ca} < 1.5$; ${}^N\text{REE} < 1.5$; $Sr > 1.5$ must be met. At this step, in some subgroups, it is possible to select series.

3.7. Synthesizing the Diagnostic Scheme

The general diagnostic scheme of minerals of the eudialyte group minerals is shown in Table 4. It can be supplemented by new members without changing its hierarchical structure. This scheme does not require writing the complete empirical formula of the mineral, but uses some rules for writing it, for example, the sequence of filling the $M(1)$ position with different elements when the calcium content is below 6 *pfu*. It is important to note that many positions in the crystal structure of EGMs (for example, $M3$ and $M4$) are filled statistically and therefore an empirical formula can only be obtained by solving the structure of the mineral. The approach we propose makes it possible, in conditions of limited data (only on chemical composition), to navigate in the virtually infinite variety of minerals of the eudialyte group.

Table 4. Calculation of formula coefficients for holotype samples of ikranite and mogovidite.

			Davinciite series * $N_{Na} > 10.5; K > 1.5;$ $N_{Ca} < 1.5; N_{REE} < 1.5; N_{Sr} < 1.5$	DAVINCIITE
		Eudialyte subgroup $4.5 \geq M^{(2)}Mn + M^{(2)}Fe > 1.5;$ $M^{(2)}Fe > M^{(2)}Mn;$ $Fe^{2+} > Fe^{3+}$		RASTSVETAEVITE
	T + T eudialytes $Si > 25.5$ $Nb \leq 0.5$ $W \leq 0.5$	Eudialyte series $N_{Na} > 13.5; K < 1.5;$ $N_{Ca} < 1.5; N_{REE} < 1.5; Sr < 1.5$	EUDIALYTE $Ti < 0.25$	
				LABYRINTHITE $Ti > 0.25$
		Fengchengite subgroup $4.5 \geq M^{(2)}Mn + M^{(2)}Fe > 1.5;$ $M^{(2)}Fe > M^{(2)}Mn;$ $Fe^{3+} > Fe^{2+}$	FENGCHENGITE $N_{Na} < 13.5; K < 1.5; N_{Ca} < 1.5;$ $N_{REE} < 1.5; Sr < 1.5$	
		Manganoeudialyte subgroup $4.5 \geq M^{(2)}Mn + M^{(2)}Fe > 1.5;$ $M^{(2)}Mn > M^{(2)}Fe$	ILYUKHINITE $N_{Na} \leq 13.5; K < 1.5; N_{Ca} < 1.5;$ $N_{REE} < 1.5; Sr < 1.5$	
		Aqualite subgroup $M^{(2)}Mn + M^{(2)}Fe \leq 1.5$	MANGANOEUDIALYTE $N_{Na} > 13.5; K < 1.5; N_{Ca} < 1.5;$ $N_{REE} < 1.5; Sr < 1.5$	
			AQUALITE $N_{Na} < 4.5; K < 1.5; N_{Ca} < 1.5; N_{REE} < 1.5; Sr < 1.5;$	
			KENTBROOKSITE $N_{Na} > 13.5; K < 1.5; N_{Ca} < 1.5;$ $N_{REE} < 1.5; Sr < 1.5; CO_3 \leq 0.5$	
		Kentbrooksite subgroup $4.5 \geq M^{(2)}Mn + M^{(2)}Fe > 1.5;$ $M^{(2)}Mn > M^{(2)}Fe$	CARBOKENTBROOKSITE $N_{Na} > 13.5; K < 1.5;$ $N_{Ca} < 1.5; N_{REE} < 1.5; Sr < 1.5; CO_3 > 0.5$	
			ANDRIANOVITE $N_{Na} > 10.5; K > 1.5; N_{Ca} < 1.5;$ $N_{REE} < 1.5; Sr < 1.5; CO_3 \leq 0.5$	
			ODIKHINCHAITE $N_{Na} > 7.5; K < 1.5; N_{Ca} < 1.5; Sr > 1.5;$ $N_{REE} < 1.5; CO_3 \leq 0.5$	
			ZIRSILITE-(Ce) $N_{Na} > 10.5; K < 1.5; N_{Ca} < 1.5;$ $N_{REE} > 1.5; Sr < 1.5; CO_3 \leq 0.5$	
	Ca-rich zirconium eudialytes $\Sigma Ca > 4.5$		FEKLICHEVITE $N_{Na} > 10.5; K < 1.5; N_{REE} < 1.5; Sr < 1.5$	
		T + Nb eudialytes $24.5 < Si \leq 25.5;$ $Nb > 0.5 \geq W$	GOLYSHEVITE $N_{Na} > 7.5; K < 1.5; N_{REE} < 1.5; Sr < 1.5$	
		Ferrokentbrooksite subgroup $4.5 \geq M^{(2)}Mn + M^{(2)}Fe > 1.5;$ $M^{(2)}Fe > M^{(2)}Mn;$	TASEQITE $N_{Na} > 10.5; K < 1.5; N_{Ca} < 1.5; N_{REE} < 1.5; Sr > 1.5;$	
			FERROKENTBROOKSITE $N_{Na} > 13.5; K < 1.5; N_{REE} < 1.5; Sr \leq 1.5$	
		Siudaite subgroup $M^{(2)}Mn + M^{(2)}Fe > 4.5;$ $Fe^{3+} > Fe^{2+}$	SIUDAITE $N_{Na} > 7.5; K < 1.5; N_{Ca} < 1.5; N_{REE} < 1.5; Sr < 1.5$	
		Georgbarsanovite subgroup $M^{(2)}Mn + M^{(2)}Fe > 4.5;$ $Fe^{2+} > Fe^{3+}$	GEORGBARSANOVITE $N_{Na} > 10.5; K < 1.5; N_{Ca} < 1.5; N_{REE} < 1.5; Sr < 1.5$	
	T + W eudialytes $24.5 < Si \leq 25.5;$ $W > 0.5 \geq Nb$	Khomyakovite subgroup $4.5 \geq M^{(2)}Mn + M^{(2)}Fe > 1.5;$ $M^{(2)}Fe^{2+} > M^{(2)}Mn$	KHOMYAKOVITE $N_{Na} > 10.5; K < 1.5; N_{Ca} < 1.5;$ $N_{REE} < 1.5; Sr > 1.5$	
		Manganokhomyakovite subgroup $4.5 \geq M^{(2)}Mn + M^{(2)}Fe > 1.5;$ $M^{(2)}Mn > M^{(2)}Fe$	JOHNSENITE-(Ce) $N_{Na} > 10.5; K < 1.5; N_{Ca} < 1.5;$ $N_{REE} > 1.5; Sr < 1.5$	
			MANGANKHOMYAKOVITE $N_{Na} > 10.5; K < 1.5;$ $N_{Ca} < 1.5; N_{REE} < 1.5; Sr > 1.5$	

Table 4. Cont.

<i>Zirconium eudialytes</i> $\Sigma Zr >$ 2.25	Ca-poor zirconium eudialytes $\Sigma Ca \leq 4.5$	T + □ eudialytes $24.5 < Si \leq 25.5;$ $Nb \leq 0.5; W \leq 0.5$	Mogovidite subgroup $4.5 \geq M^{(2)}Mn + M^{(2)}Fe > 1.5;$ $M^{(2)}Fe^{2+} > M^{(2)}Mn$	MOGOVIDITE $^N Na > 7.5; K < 1.5; ^N Ca \geq 4.5;$ $^N REE < 1.5; Sr < 1.5$
		□ + □ eudialytes $24.5 < Si \leq 25.5;$ $Nb \leq 0.5$	Ikranite subgroup $4.5 \geq M^{(2)}Mn + M^{(2)}Fe > 1.5;$ $M^{(2)}Fe > M^{(2)}Mn$	IKRANITE $^N Na < 10.5; K < 1.5; ^N Ca < 1.5; ^N REE < 1.5; Sr < 1.5$
		T + M eudialytes $24.5 < Si \leq 25.5;$ $Nb > 0.5$	Oneillite subgroup $10.5 \geq Ca + Mn + Fe > 7.5;$ $Ca > 1.5$ $M^{(1)}Mn > M^{(1)}Fe$ $M^{(2)}Fe > M^{(2)}Mn$	ONEILLITE $Na > 13.54; K < 1.5; REE < 1.5; Sr < 1.5$
		Raslakite subgroup $7.5 \geq Ca + Mn + Fe > 4.5;$ $Ca > 1.5$ $M^{(1)}Fe > M^{(1)}Mn$ $M^{(2)}Fe > M^{(2)}Mn$	RASLAKITE $Na > 16.5; K < 1.5; REE < 1.5; Sr < 1.5$	
		T + T eudialytes $Si > 25.5;$ $Nb \leq 0.5$	Sergevanite subgroup $7.5 \geq Ca + Mn + Fe > 4.5;$ $Ca > 1.5$ $M^{(1)}Mn > M^{(1)}Fe$ $M^{(2)}Fe > M^{(2)}Mn$	SERGEVANITE $Na < 13.5; K < 1.5; REE < 1.5; Sr < 1.5$
		Voronkovite subgroup $7.5 \geq Ca + Mn + Fe > 4.5;$ $Ca < 1.5$	VORONKOVITE $Na > 16.5; K < 1.5; REE < 1.5; Sr < 1.5$	
DUALITE $0.75 < \Sigma Zr \leq 2.25$ ALLUAIVITE $\Sigma Zr \leq 0.75$		* IR research is necessary. Rastsvetaevite differs from davinciite in the presence of additional splitting of bands in the IR spectrum.		

4. Conclusions

We propose a diagnostic scheme for the eudialyte-group minerals based on their chemical composition (and, in four cases, by using IR spectroscopy, for detection manganeseeudialyte, oneillite, mogovidite and ikranite). The scheme includes five consecutive steps, each of which evaluates the content of a species-forming element (or the sum of such elements). So, it is possible name any eudialyte-group mineral sample without applying a time-consuming crystallographic investigation.

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