Odikhinchaite, Na$_9$S$_3$(H$_2$O)$_2$Na$\cdot$Ca$_6$Mn$_3$Zr$_3$NbSi$_3$(Si$_{24}$O$_{72}$)O(OH)$_3$(CO$_3$)-H$_2$O, a New Eudialyte-Group Mineral from the Odikhincha Intrusion, Taimyr Peninsula, Russia

Yuliya D. Gritsenko, Nikita V. Chukanov, Sergey M. Aksenov, Igor V. Pekov, Dmitry A. Varlamov, Leonid A. Pautov, Svetlana A. Vozchikova, Dmitry A. Ksenofontov, and Sergey N. Britvin

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Abstract: The new eudialyte-group mineral, odikhinchaite, was discovered in a peralkaline pegmatite vein hosted by melteigite at the Odikhincha ultrabasic–carbonatite intrusion, Taimyr Peninsula, Krasnoyarsk Krai, Russia. Associated minerals are orthoclase, albite, aegirine, cancrinite, ancyelite-(Ce), catapleiite, and wadeite. Odikhinchaite occurs as dense rosette-like aggregates up to 11 mm across, consisting of split lamellar individuals. The mineral is translucent to transparent, deep purple, with vitreous luster. Odikhinchaite is brittle, with uneven fracture; distinct cleavage on (001) is observed. Hardness determined by the micro-indentation method is equal to 430 kgf/mm$^2$; the Mohs hardness is 5. \(D(\text{meas.)}) = 2.97(1)\text{ g cm}^{-3}\), \(D(\text{calc.)}) = 3.04\text{ g cm}^{-3}\). Odikhinchaite is optically uniaxial (-), \(\omega = 1.638(2)\), \(\epsilon = 1.630(2)\). The IR spectrum shows the presence of the $^{IV}$Mn$^{2+}$O$_4$ polyhedra, H$_2$O molecules and CO$_3^-$ anions. The chemical composition is (electron microprobe, H$_2$O determined by the modified Penfield method, CO$_2$ determined by selection sorption of gaseous annealing products; wt%): Na$_2$O 9.25, K$_2$O 0.59, CaO 12.77, MnO 5.49, FeO 0.75, MgO 0.24, La$_2$O$_3$ 0.38, Ce$_2$O$_3$ 0.39, Nd$_2$O$_3$ 0.15, Al$_2$O$_3$ 0.07, SiO$_2$ 44.80, ZrO$_2$ 11.13, TiO$_2$ 0.07, Nb$_2$O$_5$ 4.17, Cl 0.69, CO$_2$ 0.90, H$_2$O 2.22, total 99.72. The crystal structure was solved using single-crystal X-ray diffraction data. Odikhinchaite is trigonal, space group $R3m$; the unit-cell parameters are: $a = 14.2837(2)$ Å, $c = 30.0697(3)$ Å, $V = 5313.04(12)$ Å$^3$. The new mineral is isostructural with other 12-layered members of the eudialyte group with the space group $R3m$. Its crystal chemical formula is $[Z_3(Na_{2.58}Ca_{0.42})]^3[Na_{2.37}Ca_{0.51}(H_2O)_{0.12}]^{11}(Sr_{0.03}K_{0.45}Na_{0.56}REE_{0.20})^{11}Na_{3}^{N3}[H_2O_{1.8}Na_{1.2}]^{11}Zr_3 \ M_1^{M1}Ca_6^{M2}(Mn_{2.40}Fe_{2.50})^{11}M_3^{M3}Nb(OH)_{1.82}O_{1.18}[SiO_4]^{11}[SiO_2]^{X1}[CO_3]^{0.33}Cl_{0.17}^{X2}[H_2O]_{0.6}^{X3}[OSi]_{0.15}$. The strongest lines of the powder X-ray diffraction pattern $[d, \lambda, \%] (hkl)$ are: 11.42 (101), 4.309 (41) (205), 3.405 (53) (131), 3.208 (45) (208, 036), 3.167 (44) (217) 2.978 (100) (315), 2.858 (86) (404).
1. Introduction

Eudialyte was first discovered in Greenland about 200 years ago [1] and was considered as a mineral species with unstable chemical composition. Later it was supposed that eudialyte is an endmember of the “eudialyte–eucolite” solid solution, however, later, based on a chemical and X-ray structural study, it was concluded that the term “eucolite” was applied to different eudialyte-related mineral species. At present, thirty valid eudialyte-group minerals (EGMs) are distinguished [2–8].

During recent decades, EGMs attracted attention of researchers due to their remarkable set of chemical and crystal-chemical features, unique structural variability and complexity. These minerals are excellent models, demonstrating interesting complex mechanisms of homovalent, heterovalent, and, especially, blocky isomorphism involving groups of atoms that have different valence states and coordination [7,8]. These minerals are considered as geochemical markers which play an important role in the understanding of the distribution of different metals in peralkaline rocks and melts. Due to high concentrations of so-called strategic metals, EGMs are a potential source of some rare elements—first Zr, Hf and REE.

The general formula of EGM can be written as \([N1N2N3N4N5]_3\)\(_2\)\(_9\)\(_{O4}X_{12}X_{2}\), where \(Z = Zr, Ti, Nb\); \(M1 = Ca, Mn^{2+}, Fe^{3+}, Na, REE\); \(M2 = Fe^{2+}, Fe^{3+}, Mn^{2+}, Zr, Na\); \(M3-4 = Si, Nb, W\); \(N1-5 = Na, Ca, Mn, Sr, K, REE, H2O, H3O; O = OH; X = Cl, H2O, CO3\). The eudialyte-type crystal structure is based on a heteropolyhedral pseudo-framework built up by the rings of tetrahedra (Si\(_9\)O\(_{27}\) and Si\(_6\)O\(_{27}\)) and of octahedra (M\(_{16}\)O\(_{24}\)) connected via M\(_{2}O_{4-7}\) polyhedra and Z\(_{O}\)\(_{6}\) octahedra containing additional M3 and M4 sites, which are situated at the centers of two nonequivalent Si\(_9\)O\(_{27}\) rings and can be filled by additional T\(_{O4}\)-tetrahedra (predominantly occupied by silicon) or (M\(_{O}\)\(_{6}\)-octahedra (occupied by different cations having octahedral coordination) [1,2]. Five extra-framework sites, N1–5, are usually occupied by Na, but the N3 and N4 sites may contain significant and even dominant amounts of other cations (K\(^{+}\), Ca\(^{2+}\), Mn\(^{2+}\), Sr\(^{2+}\), REE\(^{3+}\)). In so-called “hydroeudialytes”, the N sites contain H\(_2\)O molecules in significant amounts [1]. The X1 and X2 sites located on the three-fold axis are occupied by extra-framework anions (Cl\(^{-}\), F\(^{-}\), OH\(^{-}\), SO\(^{2-}\), and CO\(_3^{2-}\)) and water molecules.

In this paper we describe a new eudialyte-group mineral, odikhinchaite, from the Odikhincha ultrabasic alkaline–carbonatite intrusion belonging to the Maimecha–Kotuy alkaline province. It is situated in the Kotuy river basin, at the southern part of the Taimyr Peninsula, Krasnoyarsk Krai, Polar Siberia, Russia. The specific crystal-chemical feature of this mineral, distinguishing it from other members of the eudialyte group, is the combination of \(N3Sr, N5(H2O), M2Mn^{2+}, M3Nb\), and \(X1(CO3^{2-}\)) as species-defining components.

Odikhinchaite is named after the discovery locality. The mineral and its name have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA no. 2020-064). The type specimens are deposited in the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow, Russia with the registration numbers 5587/1 and 5588/1.

2. Geological Setting

The Odikhincha ultrabasic alkaline–carbonatite complex is the second in size intrusion of the Maimecha–Kotuy alkaline province. The Odikhincha intrusion is situated at the watershed of the Medvezhya and Kotuy rivers, in the peripheral part of the Anabarsky Pre-Cambrian shield and is hosted by Cambrian dolomites [9]. The area of the modern erosional truncation of the intrusion is 56 km\(^2\).
Odikhincha is a multistage ring intrusive complex formed as a result of consecutive intrusion of olivinites, jacupirangites, melilite-bearing rocks, melteigites, and ijolites. The latest vein rocks are alkaline syenites, nepheline syenites, melanephelinites, and carbonatites. The veins are up to 3 m thick and no more than ~100 m long. Olivinites mainly occur as xenoliths typically to several hundred meters hosted by ijolites, jacupirangites and melteigites in the northern and eastern parts of the Odikhincha intrusion. Melilite-bearing rocks (okaites and turjaïtes) form two large bodies up to 9 km long in the NE part of the intrusion. Ijolites occur in the central, western and southern parts of the intrusive complex. The central part of the intrusion is predominantly composed of coarse-grained ijolites whereas medium- and fine-grained ijolites and melteigites occur in the peripheral parts of Odikhincha. Veins of alkaline syenites and nepheline syenites up to 2 m thick are the latest formations. They are confined to the peripheral parts of the complex and crosscut all other intrusive rocks. Different rocks of the intrusion host multiple lenticular bodies (up to 30 m long) and veins (up to 1 m thick) of calcite carbonatites. Pegmatoid andradite- and melilite-bearing veins with variable contents of pyroxene and nepheline are widespread too.

Outcrops of calcite carbonatite and two pegmatite veins related to nepheline syenites were found among fine-grained melteigites in the valley of the second right tributary of the Ebe-Yuryakh stream, in the southeastern part of the intrusion, 0.5–1 km from the contact with the host dolomites.

The largest pegmatite vein, 3.5 m thick, was exposed on the stream slope by four ditches. Two zones are observed in this peralkaline pegmatite body: a fine-grained zone composed of nepheline–feldspar–aegirine aggregate, with poikilitic-developed crystals of lamprophyllite and sheaf-like rinkite-(Ce) segregations, and a coarse-grained zone composed with tabular feldspar crystals up to a few centimeters in size and subordinate xenomorphic rinkite-(Ce) (lovchorrite) and lamprophyllite individuals. EGM in this pegmatite are represented only by taseqite. It forms large (up to $1 \times 0.5$ cm$^2$) light brown flattened crystals in the central part of pegmatite and is associated with lovchorrite, aegirine, orthoclase, and titanite. The ranges of main components in this mineral are: $Na_{12.3-12.4}K_{0.5}Ca_{6-6.4}Sr_{1.5-1.7}Fe_{1.9-2.4}Mn_{0.5-0.7}Nb_{0.5-0.6}Ti_{0.2-0.5}Zr_{2.5-2.7}Si_{25.3-25.5}O_{73}(O,H,O)_{1}(O,H,Cl)_{5}$ [10].

Downslope, in the stream bed, 70 m from the large pegmatite vein, another vein of peralkaline pegmatite was found among fine-grained melteigites. This thin (up to 2 cm thick) pegmatite vein was composed of coarse-crystalline orthoclase, albite, aegirine, cancrinite, and subordinate odikhinchaite.

3. Materials and Methods

Odikhinchaite occurs as dense rosette-like aggregates up to 11 mm across, consisting of split lamellar individuals (Figure 1). Along the periphery, odikhinchaite spherulites overgrow and are partially replaced by a fine-grained catapleiite aggregate, typically together with ancylite-(Ce) (Figure 2). Other associated minerals are orthoclase, albite, aegirine, cancrinite, and wadeite.

Five chemical analyses were carried out using a Tescan VEGA-II XMU INCA Energy 450, (EDS mode, 20 kV, 190 pA; TESCAN, Brno, Czech Republic). The H$_2$O was determined by means of the modified Penfield method. Selective sorption of CO$_2$ was carried out on askarite sorbent (an asbestiform matter saturated by NaOH) from gaseous products obtained by heating of the mineral at 1080 °C in oxygen flow at 1 atm.

In order to obtain IR absorption spectra of odikhinchaite and taseqite, powdered samples were mixed with anhydrous KBr, pelletized, and analyzed using an ALPHA FTIR spectrometer (Bruker Optics, Karlsruhe, Germany)) at a resolution of 4 cm$^{-1}$. Sixteen scans were collected. The IR spectrum of an analogous pellet of pure KBr was used as a reference.

Powder X-ray diffraction data were collected using a Rigaku R-AXIS Rapid II (Rigaku Corporation, Tokyo, Japan) diffractometer (image plate), CoKα, 40 kV, 15 mA, rotating anode with the microfocus optics, Debye–Scherrer geometry, $d = 127.4$ mm, exposure 15 min. The raw powder XRD data were collected using program suite designed by Britvin et al. [11]. Calculated intensities were obtained by means of STOE WinXPOW v. 2.08 program suite based on the atomic coordinates and unit-cell parameters.
Figure 1. Odikhinchaite aggregates (purple rosettes) in pegmatite with white alkali feldspars, yellow cancrite and dark green to black aegirine.

Figure 2. Fragments of odikhinchaite (Od) individuals with albite (Ab) inclusions in association with ancylite-(Ce) (Anc) and orthoclase (Or). BSE images of polished sections.

Single-crystal X-ray diffraction studies of odikhinchaite were carried out at room temperature with an Xcalibur Oxford Diffraction (Oxford Diffraction Ltd.: Abingdon, Oxfordshire, UK) diffractometer equipped with a CCD detector using the ω scanning mode. Raw data were integrated by using the CrysAlis (Oxford Diffraction Ltd.: Abingdon, Oxfordshire, UK) program [12] and then scaled, merged. A total of 27,254 reflections within the sphere limited by θ = 32.66° were measured. Based on the single crystal X-ray analysis, the following unit-cell parameters have been obtained by the least-squares refinement of all reflections: \( a = 14.2837(2) \) Å, \( c = 30.0697(3) \) Å, \( V = 5313.04(12) \) Å\(^3\). The analysis of systematic absences of reflections shows R-centering, common for eudialyte-group minerals. The space group \( R3m \) was chosen. Experimental details are given in Table 1.
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Table 1. Crystal data, data collection information and structure refinement details for odikhinchaite.

| Crystal Data                                      |
|--------------------------------------------------|
| Simplified formula                               | Na$_9$Sr$_3$[(H$_2$O)$_2$Na]Ca$_6$Mn$_3$Zr$_3$NbSi(Si$_2$O$_7$)$_2$O(OH)$_3$(CO$_3$)$_2$·H$_2$O |
| Formula weight, $M_r$ (g)                         | 3270.52                                            |
| Crystal system, space group                      | Trigonal, $R3m$ (#143)                            |
| Temperature (K)                                  | 293                                               |
| $a$, $c$ (Å)                                     | 14.2837(2), 30.0697(3)                            |
| $V$ (Å$^3$)                                      | 5313.04(12)                                       |
| $Z$                                              | 3                                                 |
| Radiation type; $\lambda$                       | MoK$\alpha$; 0.71073                              |
| Absorption coefficient, $\mu$ (mm$^{-1}$)        | 3.91                                              |
| Crystal size (mm)                                | 0.3 × 0.1 × 0.05                                  |

| Data Collection                                  |
|--------------------------------------------------|
| Diffractometer                                   | Xcalibur, Sapphire3 (CCD detector)                |
| Absorption correction                            | Multi scan                                        |
| $T_{\text{min}}, T_{\text{max}}$                 | 0.773; 1                                           |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 27,254, 2345, 2312                                 |
| $R_{\text{int}}$                                  | 0.053                                             |
| $(\sin \theta/\lambda)_{\text{max}}$ (Å$^{-1}$)  | 0.759                                             |

| Refinement                                        |
|--------------------------------------------------|
| Refinement on                                    | Full-matrix least squares on $F$                  |
| $R[I > 2\sigma(I)]$, $wR(I)$, $S$                 | 0.031, 0.043, 1.63                                |
| Weight scheme                                    | $1/(\sigma^2|F| + 0.0004F^2)$                     |
| No. of refinement parameters ($N_{\text{par}}$)   | 265                                               |
| $N_{\text{ref}}/N_{\text{par}}$                  | 8.73                                              |
| $\Delta \rho_{\text{max}}, \Delta \rho_{\text{min}}$ (e Å$^{-3}$) | −1.25/1.10                                       |

4. Results

4.1. Physical Properties

Odikhinchaite is translucent to transparent, deep purple, with vitreous luster. The streak is white. The new mineral is brittle, with uneven fracture; distinct cleavage on (001) is observed. Hardness determined by the micro-indentation method (the Vickers hardness number $= VHN$, load 20 g) is equal to 430 kgf/mm$^2$ (range 394–491, $n = 6$). The Mohs hardness is 5. Density measured by flotation in heavy liquids (mixtures of methylene iodide and benzene) is 2.97(1) g cm$^{-3}$. Density calculated using the empirical formula and unit cell volume refined from single crystal XRD data is 3.04 g cm$^{-3}$.

4.2. Infrared Spectroscopy

Absorption bands in the IR spectrum of odikhinchaite (curve a in Figure 2) and their assignments are (cm$^{-1}$; s—strong band, w—weak band, sh—shoulder): 3435, 3220sh (O–H stretching vibrations), 1635w (H–O–H bending vibrations), 1507w, 1451, 1407w (asymmetric stretching vibrations of the CO$_3^{2-}$ groups), 1060sh, 1016s, 975s, 923s (Si–O stretching vibrations), 740, (mixed vibrations of tetrahedral rings—“ring band”), 697w, 662 (mixed vibrations of tetrahedral rings combined with Nb–O stretching vibrations), 545sh (IV Fe$^{2+}$–O stretching vibrations), 526 (IV Mn$^{2+}$–O stretching vibrations), 479s, 453s.
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(lattice mode involving predominantly bending vibrations of tetrahedral rings), 390, 364 (lattice modes involving Ca–O stretching vibrations). The assignment of IR bands was made based on the analysis of IR spectra of several tens structurally investigated eudialyte-group minerals, in accordance with [1].

The IR spectrum of odikhinchaite differs from that of its $M^2Fe^{2+}$-dominant and CO$_2$-deficient analogue taseqite with the crystal-chemical formula [Na$_{10.5}$K$_{0.5}$(Sr$_{1.71}$Na$_{1.29}$)] [Ca$_{5.85}$REE$_{0.15}$]Zr$_{2.96}$Hf$_{0.03}$[Fe$_{2.43}$Mn$_{0.45}$]Si$_2$(Nb$_{0.64}$Ti$_{0.27}$)$(Si_3O_9)_2$$(Si_3O_9)_2$(OH,CO$_3$)$_3$ from the Odikhincha massif (curve b on Figure 3) in higher intensities of the bands of O–H, C–O, Nb–O and IV$^{4+}$Mn$^{2+}$–O stretching vibrations and a lower intensity of the band of IV$^{4+}$Fe$^{2+}$–O stretching vibrations, which is in accordance with crystal-chemical features of these minerals.

Figure 3. Powder infrared absorption spectra of (a) odikhinchaite and (b) taseqite, both from the Odikhincha alkaline complex.

4.3. Optical Properties

Odikhinchaite is optically uniaxial (−), $\omega = 1.638(2)$, $\varepsilon = 1.630(2)$ ($\lambda = 589$ nm). Under the microscope, the mineral is strongly pleochroic: $O =$ bright crimson, $E =$ light yellow. The absorption scheme is: $O > E$.

4.4. Chemical Composition

Chemical data for odikhinchaite are given in Table 2. Contents of other elements with atomic numbers > 8 are below detection limits.

The formula coefficients based on 29 high force-strength framework cations, i.e., Si + Al + Nb + Zr + Ti atoms per formula unit (apfu, for $Z = 3$), in accordance with structural data are H$_{0.22}$Na$_{0.97}$K$_{0.42}$Ca$_{7.59}$Sr$_{1.87}$Ce$_{0.08}$La$_{0.08}$Nd$_{0.03}$Mn$_{2.58}$Fe$_{0.35}$Mg$_{0.20}$Ti$_{0.02}$Zr$_{3.01}$Nb$_{0.10}$Si$_{24.87}$Al$_{0.05}$Cl$_{0.65}$C$_{0.68}$O$_{81.71}$.

The end-member formula is Na$_9$Sr$_3$[(H$_2$O)$_2$Na]Ca$_6$Mn$_3$Zr$_3$NbSi(Si$_2$O$_7$)$_3$(OH)$_3$(CO$_3$)$_2$·H$_2$O.

The compatibility index $1−(K_p/K_c)$ is equal to −0.005 (superior) with density calculated using the crystal-chemical formula and −0.024 (excellent) with measured density.
Table 2. Chemical data for odikhinchaite.

| Constituent | Mean Content, wt% | Range | Standard Deviation | Probe Standard |
|-------------|-------------------|-------|--------------------|----------------|
| Na₂O       | 9.26              | 8.97–9.68 | 0.29             | Albite         |
| K₂O        | 0.59              | 0.41–0.76 | 0.24             | Orthoclase     |
| CaO        | 12.77             | 12.42–13.58 | 0.15            | Wollastonite   |
| MnO        | 5.49              | 5.21–6.49 | 0.18             | Mn             |
| FeO        | 0.75              | 0–1.26   | 0.13             | Fe             |
| MgO        | 0.24              | 0.08–0.35 | 0.14             | MgO            |
| SrO        | 5.81              | 4.55–6.63 | 0.09             | SrF₂           |
| La₂O₃      | 0.38              | 0.11–0.63 | 0.12             | LaPO₄          |
| Ce₂O₃      | 0.39              | 0–1.41   | 0.15             | CePO₄          |
| Nd₂O₃      | 0.15              | 0–0.42   | 0.21             | NdPO₄          |
| Al₂O₃      | 0.07              | 0–0.17   | 0.11             | Albite         |
| SiO₂       | 44.80             | 44.12–45.74 | 0.74           | SiO₂           |
| ZrO₂       | 11.13             | 10.82–11.72 | 0.19          | Zr             |
| TiO₂       | 0.07              | 0–0.41   | 0.14             | Ti             |
| Nb₂O₅      | 4.17              | 3.21–4.74 | 0.21             | Nb             |
| Cl         | 0.69              | 0.61–0.83 | 0.02             | NaCl           |
| CO₂        | 0.90              | -       | -                | -              |
| H₂O        | 2.22              | -       | -                | -              |
| -O = Cl    | -0.16             | -       | -                | -              |
| Total      | 99.72             | -       | -                | -              |

4.5. X-Ray Diffraction Data and Crystal Structure

Powder X-ray diffraction data are presented in Table 3. Diffraction peaks are readily indexed in the space group R₃m. The unit-cell parameters calculated from the powder data are: \( a = 14.2179(1) \), \( c = 30.3492(3) \) Å, \( V = 5313.1(1) \) Å³.

Table 3. Powder X-ray diffraction data (\( d \) in Å) of odikhinchaite.

| \( I_{\text{obs}} \) | \( d_{\text{obs}} \) | \( I_{\text{calc}} * \) | \( d_{\text{calc}} ** \) | \( h k l \) | \( I_{\text{obs}} \) | \( d_{\text{obs}} \) | \( I_{\text{calc}} * \) | \( d_{\text{calc}} ** \) | \( h k l \) |
|---------------------|---------------------|---------------------|---------------------|--------|---------------------|---------------------|---------------------|---------------------|--------|
| 64                  | 11.42               | 100                 | 11.439              | 101    | 17                  | 2.138               | 4                    | 2.144               | 0.57    |
| 9                   | 10.01               | 12                  | 10.023              | 003    | 2                   | 2.085               | 3                    | 2.084               | 155     |
| 36                  | 9.54                | 51                  | 9.552               | 012    | 7                   | 2.118               | 6                    | 2.116               | 0.1.14  |
| 24                  | 7.13                | 15                  | 7.142               | 110    | 3                   | 2.098               | 4                    | 2.100               | 149     |
| 38                  | 6.42                | 23                  | 6.424               | 104    | 9                   | 2.062               | 6                    | 2.064               | 3.2.10  |
| 24                  |                     |                     |                     |        |                     |                     |                     |                     |        |
| 24                  | 6.05                | 22                  | 6.058               | 021    | 8                   | 2.055               | 5                    | 2.053               | 247     |
| 39                  | 5.71                | 26                  | 5.720               | 202    | 4                   | 2.027               | 5                    | 2.029               | 431     |
Table 3. Cont.

| $I_{\text{obs}}$ | $d_{\text{obs}}$ | $I_{\text{calc}}$* | $d_{\text{calc}}$** | $h\ k\ l$ | $I_{\text{obs}}$ | $d_{\text{calc}}$* | $d_{\text{calc}}$** | $h\ k\ l$ |
|------------------|------------------|--------------------|--------------------|---------|------------------|--------------------|--------------------|---------|
| 3                | 5.42             | 1                  | 5.409              | 015     | 6                | 2.019              | 2.015              | 603     |
| 6                | 5.01             | 6                  | 5.012              | 006     | 19               | 1.984              | 1.981              | 428     |
| 3                | 4.774            | 2                  | 4.776              | 024     | 3                | 1.952              | 1.952              | 1.214   |
| 3                | 4.611            | 3                  | 4.620              | 211     | 9                | 1.938              | 019              | 339     |
| 41               | 4.309            | 22                 | 4.312              | 025     | 6                | 1.918              | 019              | 1.313   |
| 19               | 4.100            | 13                 | 4.102              | 116     | 13               | 1.907              | 1.907              | 0.510   |
| 25               | 3.967            | 22                 | 3.970              | 214     | 3                | 1.881              | 1.883              | 161     |
| 19               | 3.810            | 11                 | 3.813              | 303     | 3                | 1.872              | 2.872              | 612     |
| 7                | 3.689            | 7                  | 3.691              | 125     | 4                | 1.856              | 2.856              | 1.856   |
| 28               | 3.567            | 7                  | 3.596              | 018     | 20               | 1.839              | 1.839              | 1.839   |
| 30               | 3.529            | 19                 | 3.528              | 027     | 8                | 1.798              | 1.798              | 1.798   |
| 53               | 3.405            | 46                 | 3.409              | 131     | 27               | 1.785              | 1.777              | 4.211   |
| 15               | 3.344            | 9                  | 3.345              | 312     | 13               | 1.764              | 1.764              | 1.764   |
| 45               | 3.208            | 37                 | 3.212              | 208     | 6                | 1.749              | 1.749              | 1.749   |
| 44               | 3.167            | 36                 | 3.163              | 217     | 7                | 1.722              | 1.722              | 1.722   |
| 3                | 3.121            | 6                  | 3.121              | 134     | 8                | 1.713              | 1.713              | 1.713   |
| 31               | 3.025            | 12                 | 3.029              | 042     | 7                | 1.704              | 1.704              | 1.704   |
| 100              | 2.978            | 91                 | 2.980              | 315     | 12               | 1.682              | 1.682              | 1.682   |
| 21               | 2.908            | 18                 | 2.908              | 226     | 2                | 1.670              | 1.670              | 1.670   |
| 86               | 2.858            | 74                 | 2.860              | 404     | 10               | 1.647              | 1.647              | 1.647   |
Table 3. Cont.

| $i_{\text{obs}}$ | $d_{\text{obs}}$ | $d_{\text{calc}}^*$ | $d_{\text{calc}}^{**}$ | $h$ | $k$ | $l$ | $d_{\text{obs}}$ | $d_{\text{calc}}^*$ | $d_{\text{calc}}^{**}$ | $h$ | $k$ | $l$ |
|-----------------|-----------------|-----------------|-----------------|-----|-----|-----|-----------------|-----------------|-----------------|-----|-----|-----|
| 5               | 2.787           | 7               | 2.789           | 232 | 5   | 1.627|                 | 2               | 1.631           | 3.411|     |     |
|                 |                 |                 |                 |     |     |     |                 | 4               | 1.627           | 1.118|     |     |
|                 |                 |                 |                 |     |     |     |                 | 1               | 1.622           | 5.014|     |     |
| 3               | 2.747           | 4               | 2.750           | 045 | 14  | 1.606|                 | 2               | 1.609           | 4.115|     |     |
|                 |                 |                 |                 |     |     |     |                 | 13              | 1.606           | 4.016|     |     |
| 19              | 2.699           | 11              | 2.704           | 0.2.10 | 10 | 1.596|                 |                 |                 | 3   | 1.599| 538 |
|                 |                 | 7               | 2.699           | 410  | 10  | 1.596|                 |                 |                 | 6   | 1.598| 1.610|
|                 |                 | 8               | 2.681           | 137  |     |     |                 |                 |                 | 4   | 1.593| 627 |
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 1   | 1.592| 0.612|
| 12              | 2.654           | 11              | 2.655           | 324  | 4   | 1.581|                 |                 |                 | 5   | 1.582| 541 |
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 3   | 1.575| 452 |
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 1   | 1.575| 449 |
| 30              | 2.595           | 3               | 2.607           | 143  | 7   | 1.567|                 |                 |                 | 6   | 1.567| 3.216|
|                 |                 | 32              | 2.596           | 309  |     |     |                 |                 |                 |     |     |     |
| 13              | 2.530           | 8               | 2.534           | 318  | 9   | 1.552|                 |                 |                 | 4   | 1.558| 630 |
|                 |                 | 7               | 2.529           | 2.1.10 |     |     |                 |                 |                 | 2   | 1.557| 176 |
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 5   | 1.554| 2.512|
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 1   | 1.553| 6.11|
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 3   | 1.550| 544 |
| 7               | 2.508           | 5               | 2.510           | 407  | 8   | 1.546|                 |                 |                 | 1   | 1.548| 0.318|
|                 |                 | 3               | 2.506           | 0.0.12 |     |     |                 |                 |                 | 6   | 1.544| 081 |
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 1   | 1.540| 363 |
| 8               | 2.464           | 7               | 2.466           | 051  | 3   | 1.527|                 |                 |                 | 3   | 1.527| 4.313|
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 1   | 1.524| 3.510|
| 5               | 2.439           | 1               | 2.444           | 502  | 1   | 1.513|                 |                 |                 | 1   | 1.514| 084 |
|                 |                 | 3               | 2.440           | 229  |     |     |                 |                 |                 | 1   | 1.513| 2.218|
| 19              | 2.378           | 5               | 2.388           | 048  | 3   | 1.497|                 |                 |                 | 2   | 1.497| 0.516|
|                 |                 | 9               | 2.380           | 330  |     |     |                 |                 |                 | 1   | 1.493| 0.120|
|                 |                 | 9               | 2.377           | 416  |     |     |                 |                 |                 |     |     |     |
| 13              | 2.329           | 13              | 2.331           | 241  | 11  | 1.484|                 |                 |                 | 2   | 1.486| 547 |
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 8   | 1.484| 0.711|
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 2   | 1.482| 274 |
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 4   | 1.477| 3.414|
| 6               | 2.264           | 3               | 2.265           | 238  | 5   | 1.465|                 |                 |                 | 2   | 1.466| 725 |
|                 |                 | 2               | 2.261           | 1.3.10 |     |     |                 |                 |                 | 3   | 1.465| 2.416|
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 2   | 1.460| 458 |
| 3               | 2.213           | 4               | 2.216           | 511  | 2   | 1.454|                 |                 |                 | 1   | 1.454| 4.412|
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 1   | 1.453| 2.611|
| 7               | 2.196           | 7               | 2.198           | 152  | 5   | 1.437|                 |                 |                 | 3   | 1.437| 0.615|
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 1   | 1.437| 1.319|
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 1   | 1.435| 5.116|
| 6               | 2.178           | 5               | 2.179           | 425  | 9   | 1.430|                 |                 |                 | 1   | 1.420| 4.118|
|                 |                 |                 |                 |     |     |     |                 |                 |                 | 2   | 1.413| 642 |
| 16              | 2.154           | 10              | 2.156           | 4.0.10 |     |     |                 |                 |                 | 5   | 1.417| 461 |
|                 |                 | 2               | 2.150           | 336  |     |     |                 |                 |                 | 5   | 1.417| 461 |

* For the calculated pattern, only reflections with intensities $\geq 1$ are given. ** For the unit-cell parameters calculated from single-crystal data.
The structure determination and refinement of odikhinchaite were carried out based on 2312 independent reflections with \( I > 2\sigma(I) \) using the program JANA2006 (Institute of Physics, Praha, Czech Republic) \([13]\). Extra-framework sites including split and partially occupied ones have been localized from a series of difference electron-density maps calculations. Atomic scattering factors for neutral atoms together with anomalous dispersion corrections were taken from International Tables for Crystallography \([14]\). Illustrations were produced with the JANA2006 program package in combination with the program DIAMOND, Version 3 (Crystal Impact GbR, Bonn, Germany) \([15]\).

Table 4 lists the fractional atomic coordinates, site multiplicities, atomic displacement parameters and site occupancies. Selected interatomic distances are given in Table 5.

**Table 4.** Atom coordinates \((x, y, z)\), atomic displacement parameters \((U, \text{Å}^2)\), site multiplicities \((\text{Mult})\), site occupancies and bond-valence sums (BVS) in the structure of odikhinchaite.

| Site  | \(x\)     | \(y\)     | \(z\)     | \(U_{\text{iso}}^*/U_{\text{eq}}\) | \(\text{Mult}\) | Occupancy | BVS  |
|-------|------------|------------|------------|----------------------------------|----------------|-----------|-------|
| Z     | 0.16245(2) | 0.32489(5) | 0.13811(4) | 0.0066(2)                        | 9              | Zr        | 4.01  |
| M1    | −0.00293(8) | 0.2588(1)  | 0.30584(5) | 0.0089(3)                        | 18             | Ca        | 2.05  |
| Si1   | 0.07001(7)  | 0.1400(1)  | 0.22528(7) | 0.0077(5)                        | 9              | Si        | 3.98  |
| Si2   | −0.07891(14)| 0.46054(7) | 0.05013(7) | 0.0074(5)                        | 9              | Si        | 3.92  |
| Si3   | −0.05666(10)| 0.2693(1)  | 0.06888(6) | 0.0071(4)                        | 18             | Si        | 3.97  |
| Si4   | 0.26280(7)  | 0.5256(1)  | 0.05556(7) | 0.0072(5)                        | 9              | Si        | 4.11  |
| Si5   | 0.41983(15)| 0.20992(8) | 0.23062(7) | 0.0098(5)                        | 9              | Si        | 4.18  |
| Si6   | 0.39110(10)| 0.3957(1)  | 0.20748(5) | 0.0078(4)                        | 18             | Si        | 4.11  |
| O1    | −0.1813(2)  | 0.1813(2)  | 0.0858(2)  | 0.0106(14)                       | 9              | O         | -     |
| O2    | 0.0245(3)   | 0.2497(3)  | 0.0990(1)  | 0.0151(13)                       | 18             | O         | -     |
| O3    | 0.1174(2)   | 0.2349(4)  | 0.2615(2)  | 0.0127(15)                       | 9              | O         | -     |
| O4    | 0.2335(2)   | 0.4671(5)  | 0.1031(2)  | 0.0199(18)                       | 9              | O         | -     |
| O5    | 0.3578(4)   | 0.1789(2)  | 0.2768(2)  | 0.0137(16)                       | 9              | O         | -     |
| O6    | −0.2081(4)  | 0.3960(2)  | 0.0555(2)  | 0.0148(15)                       | 9              | O         | -     |
| O7    | 0.3757(3)   | 0.4102(3)  | 0.2595(1)  | 0.0139(13)                       | 18             | O         | -     |
| O8    | 0.2099(4)   | 0.6050(2)  | 0.0542(2)  | 0.0123(14)                       | 8              | O         | -     |
| O9    | 0.3876(4)   | 0.2816(3)  | 0.1985(1)  | 0.0206(16)                       | 18             | O         | -     |
| O10   | 0.0905(2)   | 0.1809(4)  | 0.1746(2)  | 0.0159(16)                       | 9              | O         | -     |
| O11   | −0.0472(3)  | 0.2548(3)  | 0.0167(1)  | 0.0153(13)                       | 18             | O         | -     |
| O12   | −0.0340(4)  | 0.4830(2)  | 0.0003(2)  | 0.0094(14)                       | 9              | O         | -     |
| O13   | −0.0338(3)  | 0.3921(3)  | 0.0792(1)  | 0.0112(12)                       | 18             | O         | -     |
| O14   | 0.5067(2)   | 0.4933(2)  | 0.1892(2)  | 0.0130(15)                       | 9              | O         | -     |
| O15   | −0.0616(2)  | 0.0616(2)  | 0.2322(2)  | 0.0137(15)                       | 9              | O         | -     |
| O16   | 0.2981(3)   | 0.3975(3)  | 0.1793(2)  | 0.0194(14)                       | 18             | O         | -     |
| O17   | 0.2234(2)   | 0.4468(5)  | 0.0149(2)  | 0.0179(18)                       | 9              | O         | -     |
| O18   | 0.5462(5)   | 0.2731(2)  | 0.2387(2)  | 0.036(2)                         | 9              | O         | -     |
| M2    | 0.4832(1)   | 0.5168(1)  | 0.3077(5)  | 0.0122(3)                        | 9              | Mn_{0.83}Fe_{0.17} | 2.10 |
| M3    | 1/3        | 2/3        | 0.34260(5) | 0.0114(2)                        | 3              | Nb        | 5.06  |
| OH\(^{M3}\) | 0.3981(2)  | 0.6019(2)  | 0.3092(2)  | 0.0162(15)                       | 9              | (OH)_{0.66}O_{0.39} | -   |
| M4a   | 0          | 0          | 0.8834(1)  | 0.0093(8)                        | 3              | Si_{0.82} | -     |
| OH\(^{M4a}\) | 0          | 0          | 0.8303(4)  | 0.016(3)                         | 3              | (OH)_{0.82} | -   |
Table 4. Cont.

| Site  | x      | y      | z      | Uiso* | Ueq | Mult | Occupancy | BVS |
|-------|--------|--------|--------|-------|-----|------|-----------|-----|
| M4b   | 0      | 0      | 0.9192(7) | 0.026(6) | 3   | Si0.18 | -         |
| OHM44b| 0      | 0      | 0.975(2) | 0.0612(6)* | 3   | (OH)0.18 | -         |
| N1    | 0.4366(2) | 0.5634(5) | 0.1300(1) | 0.0299(9) | 9   | Na0.79Ca0.17(H2O)0.04 | -         |
| N2a   | -0.1093(3) | 0.1093(3) | 0.1525(2) | 0.0415(17) | 9   | Na0.86 | -         |
| N2b   | -0.0782(7) | 0.0782(7) | 0.1343(6) | 0.033(4) | 9   | Ca0.14 | -         |
| N3a   | 0.23412(1) | 0.46830(7) | 0.25630(4) | 0.0167(2) | 9   | Sr0.667K0.15Ca0.067 | -         |
| N3b   | 0.2357(14) | 0.4713(3) | 0.2267(12) | 0.0317(7)* | 9   | Na0.116 | -         |
| N4    | 0.1018(4) | 0.2036(8) | 0.0182(2) | 0.084(5) | 9   | Na     | -         |
| N5    | -0.2630(2) | 0.2630(2) | 0.1180(2) | 0.037(2) | 9   | (H2O)0.6Na0.4 | -         |
| X1a   | 1/3    | 2/3    | 0.2027(3) | 0.0237(17) | 3   | C0.53Cl0.35 | -         |
| OCX1a | 0.3827(3) | 0.6173(3) | 0.2125(8) | 0.091(8)* | 9   | O0.53 | -         |
| X1b   | 1/3    | 2/3    | 0.1541(13) | 0.0397(7)* | 3   | Cl0.12 | -         |
| X2a   | 0      | 0      | 0.0556(12) | 0.056(10) | 3   | (H2O)0.6 | -         |
| X2b   | 0      | 0      | 0.0898(18) | 0.06412(2)* | 3   | (OH,F)0.4 | -         |
| CXM4  | 0      | 0      | 0.997(8) | 0.057(12)* | C0.15 | -         |
| OCXM4 | -0.0509(2) | 0.0509(2) | 0.9993(3) | 0.08(2)* | O0.15 | -         |

Note: *Uiso; Bond-valence sums were calculated using the bond-valence parameters for the Zr4+–O, Mn2+–O, Fe2+–O, and Nb5+–O bonds [16], as well as Si4+–O bond [17]. Due to the complex coordination environments of the oxygen O1–O18 atoms (which are surrounded by partially occupied extra-framework sites) and extra-framework cations and their ligands (which are mostly partially occupied), the BVS are given only for fully occupied cationic sites.

Table 5. Selected interatomic distances (Å) in the structure of odikhinchaite.

| Bond | Distance | Bond | Distance |
|------|----------|------|----------|
| Z    | O4 2.050(6) | O14 2.484(6) |
|      | O2 × 2 2.074(5) | O8 2.500(7) |
|      | O16 × 2 2.086(4) | O4 2.639(7) |
|      | O10 2.093(5) | O4 2.641(4) |
|      | - 2.077 | O16 × 2 2.652(4) |
|      | O17 2.287(5) | X1b 2.655(11) |
|      | O3 2.332(5) | OCX1a 2.816(22) |
| M1   | O5 2.348(5) | O13 × 2 2.823(5) |
|      | O11 2.378(5) | - 2.651 |
|      | O7 2.397(4) | O2 × 2 2.536(6) |
|      | O12 2.464(5) | O10 2.590(7) |
|      | - 2.368 | O10 2.591(5) |
| Si1  | O3 1.601(5) | O15 2.671(8) |
|      | O10 1.605(6) | O1 2.683(7) |
|      | O15 × 2 1.651(4) | O9 × 2 2.802(7) |
|      | - 1.627 | - 2.651 |
**Table 5. Cont.**

| Bond   | Distance | Bond   | Distance |
|--------|----------|--------|----------|
| Si2    |          | N2b    |          |
| O12    | 1.598(5) | N1b    | 0.945(16)|
| O6     | 1.606(5) | X2b    | 2.352(34)|
| O13    | 1.663(5) | O2 × 2 | 2.385(11)|
| O13    | 1.663(4) | O10    | 2.427(12)|
|        |          | O10    | 2.428(12)|
| Si3    |          |        |          |
| O11    | 1.599(4) | O1      | 2.938(15)|
| O2     | 1.603(5) | O15     | 2.973(19)|
| O13    | 1.645(5) | X2a     | 3.057(32)|
| O1     | 1.665(3) |        |          |
|        |          |        |          |
| Si4    |          | N3a    |          |
| O17    | 1.565(6) | O7 × 2 | 2.542(4)|
| O4     | 1.602(6) | O12     | 2.639(5)|
| O8     | 1.647(5) | OHM3 × 2| 2.681(5)|
| O8     | 1.648(6) | O16 × 2 | 2.854(5)|
|        |          | O3      | 2.891(5)|
| Si5    |          | N3b    |          |
| O18    | 1.582(7) | X1a    | 2.936(5)|
| O5     | 1.587(6) |        |          |
| O9     | 1.633(6) |        |          |
|        |          | N3b    | 0.891(36)|
|        |          |        |          |
| Si6    |          | N3b    |          |
| O16    | 1.588(5) | O16    | 2.206(34)|
| O7     | 1.608(4) | O16    | 2.210(27)|
| O9     | 1.627(5) | X1a    | 2.526(37)|
| O14    | 1.635(3) | O7     | 2.732(37)|
|        |          | O7     | 2.737(24)|
|        |          |        | 2.384    |
|        |          |        |          |
| M2     |          | N4     |          |
| OHM3   | 2.105(4) | OCXM4 × 2| 2.256(24)|
| O7 × 2 | 2.106(4) | O11 × 2 | 2.574(11)|
| O11 × 2| 2.113(4) | O5      | 2.597(9)|
|        |          | X2a    | 2.758(17)|
|        |          |        |          |
| M3     |          |        |          |
| OHM3 × 3| 1.891(4)| OHM4b  | 2.835(9)|
| O6 × 3 | 2.081(6) | O2 × 2  | 2.878(9)|
|        |          | O17    | 3.010(12)|
|        |          |        |          |
| M4a    |          |        |          |
| OHM4a  | 1.598(13)|              |          |
| O18 × 3| 1.630(4) |          |          |
|        |          | O1     | 2.217(9)|
|        |          | O1     | 2.241(6)|
|        |          | O6 × 2 | 2.503(6)|
| M4b    | 1.076(22)|          |          |
Table 5. Cont.

| Bond     | Distance  | Bond     | Distance  |
|----------|-----------|----------|-----------|
| M4b      | 1.547(8)  | N5 × 2   | 3.014(5)  |
| O\textsuperscript{M4b} | 1.675(21)| O13 × 2  | 3.072(5)  |
|          | -         | -        | -         |
| X1a      | 1.256(7)  | X\textsuperscript{M4} | 1.260(5)  |
|          | 1.461(40) |          |           |

Odikhinchaite is isostructural with other 12-layered members of the eudialyte group with the space group R\textsuperscript{3}m, which is most common for eudialyte-group minerals (see Figures 4 and 5). Based on the refined site-scattering factors, the crystal chemical formula of odikhinchaite can be written as follows (Z = 3): \{N\textsuperscript{1}[Na\textsubscript{2.58}Ca\textsubscript{0.42}]\textsuperscript{N2}Na\textsubscript{2.37}Ca\textsubscript{0.51}(H\textsubscript{2}O)\textsubscript{0.12}]\textsuperscript{N3}(Sr\textsubscript{2.00}K\textsubscript{0.45}Na\textsubscript{0.35}REE\textsubscript{0.20})\textsuperscript{N4}Na\textsubscript{3}\textsuperscript{N5}[(H\textsubscript{2}O)\textsubscript{1.8}Na\textsubscript{1.2}][Z\textsuperscript{2}M3Ca\textsubscript{6}M\textsubscript{2}(Mn\textsubscript{2.49}Fe\textsubscript{2+}0.51)]\textsuperscript{M3}Nb(O\textsubscript{1.82}O\textsubscript{1.18})\textsuperscript{M4}(\textsuperscript{M4}SiOH)[\textsuperscript{Si\textsubscript{5}O\textsubscript{9}}][\textsuperscript{Si\textsubscript{9}O\textsubscript{27}}]\textsuperscript{X1}[(\textsuperscript{CO\textsubscript{3}})\textsubscript{0.53}Cl\textsubscript{0.47}]\textsuperscript{X2}[(\textsuperscript{H\textsubscript{2}O})\textsubscript{0.6}(O,F)\textsubscript{0.4}]\textsuperscript{X\textsuperscript{M4}}(\textsuperscript{CO\textsubscript{3}})\textsubscript{0.15} where braces and brackets enclose contents of the key sites.

In the crystal structure of odikhinchaite, manganese (2.49 apfu) predominates over iron(II) (0.51 apfu) at the M2-site, which is located in the center of the M2ϕ\textsubscript{5}-square pyramids (ϕ = O\textsuperscript{2−}, OH\textsuperscript{−}) with the mean distance <M2−ϕ> = 2.109 Å. The octahedral M3 site (the mean distance <M3−ϕ> = 1.986 Å) located on the threefold axis at the center of one nine-membered Si\textsubscript{9}O\textsubscript{27}-tetrahedral ring is occupied by niobium (1 apfu) while the M4 site located at the center of the symmetrically non-equivalent nine-membered tetrahedral ring is split into two M4a- and M4b-sites (M4a–M4b = 1.076 Å) occupied by silicon (0.82 and 0.18 apfu, respectively) in tetrahedral environment (the mean distances are: <M4a−ϕ> = 1.622 Å; <M4b−ϕ> = 1.579 Å). The M3ϕ\textsubscript{6} octahedron links with the M2ϕ\textsubscript{6} square pyramid via the common OH\textsuperscript{M3}-vertex forming a heteropolyhedral [NbMn\textsubscript{3}(OH,O)\textsubscript{3}] cluster (Figure 6).

Figure 4. The general view of the crystal structure of odikhinchaite (the unit cell is outlined).
Figure 5. Heteropolyhedral layer involving rings of CaO$_6$ octahedra in the structure of odikhinchaite.

Figure 6. Local coordinational environments of the N3a site (a), the X1 site (b), and the X2 site (c).

The distribution of large cations over the N1–5 sites in odikhinchaite is similar to that in taseqite [16] and its Cl-deficient variety [10]. The N1 site is split into two sites with the distance N1a–N1b = 0.945 Å. The N1a is occupied by sodium (2.58 apfu), while N1b is occupied by calcium (0.42 apfu). The N2 site has a complex composition with the predominance of sodium (2.37 apfu) and admixture of calcium (0.51 apfu) and water molecules (0.12 molecules pfu). The N4 site is fully occupied by sodium. The N5 site is predominantly occupied by water molecules (1.8 apfu) and sodium (1.2 apfu). The most distinguished feature of odikhinchaite and taseqite [10,16] is the predominance of strontium at the N3 site. In the structure of odikhinchaite, the N3 is split into two sites with the distance N3a–N3b = 0.891 Å. The N3a site has a complex chemical composition with the predominance of strontium (2.00 apfu) and admixture of potassium (0.45 apfu) and rare-earth elements (0.20 apfu) and has a variable coordination number (8 or 10 in the cases when the X1a site contains Cl$^-$ or CO$_3^{2-}$, respectively) (Figure 6a). The N3b site is occupied by sodium (0.35 apfu).

Odikhinchaite is characterized by the considerable amount of CO$_3^{2-}$ anions (0.68 anions pfu in total) which are located at the at the X sites, on the threefold axis (Figure 6b,c). It was found that CO$_3^{2-}$ group predominates over chlorine at the X1 site, which is split into two sites with the distance X1a–X1b = 1.461 Å. The X1a is occupied by CO$_3^{2-}$ (0.53 anions pfu) with admixture of chlorine (0.35 apfu), while the X1b site is occupied only by chlorine (0.12 apfu). The X2 site is also split into two sites with the distance X2a–X2b = 1.028 Å. The X2a site is occupied by water molecules (0.6 apfu) and the X2b site is occupied by the mix of hydroxyl group and fluorine atoms (0.4 apfu). Additional amount of the CO$_3^{2-}$ groups (0.15 apfu) were also localized at the X$^M4$ site between the X2a and OH$^{M4b}$ sites with the distances X$^M4$–X2a = 1.762 Å and X$^M4$–OH$^{M4a}$ = 0.662 Å.
5. Discussion

Odikhinchaite Na$_{19}$Sr$_3$[(H$_2$O)$_2$Na]Ca$_6$Mn$_3$Zr$_3$NbSi(Si$_2$O$_7$)O(OH)$_3$SiO$_3$H$_2$O belongs to the eudialyte group and adopts the eudialyte structure type. It is closely related to taseqite whose end-member formula is Na$_{12}$Sr$_3$Ca$_2$Fe$^{2+}_2$Zr$_3$NbSi(Si$_2$O$_7$)O(OH)$_3$SiO$_3$H$_2$O [18]. Unlike taseqite, which is Fe$^{2+}$-dominant at the M2 site, in odikhinchaite, this site is predominantly populated by Mn$^{2+}$. In addition, in odikhinchaite, the X2 site is predominantly occupied by the CO$_3^{2-}$ groups, whereas in taseqite, this site is Cl-dominant, and the N5 site of odikhinchaite is predominantly populated by H$_2$O.

Odikhinchaite can also be the [Na$_3$, Sr$_{15}$H$_2$O] analogue of carbokentbrooksite (Na$_2$RE$_3$Mn$_3$Zr$_3$NbSi$_2$O$_7$)O(OH)$_3$SiO$_3$H$_2$O [19] and the [M$_3$Nb, Na$_{15}$H$_2$O] analogue of manganokhomyakovite Na$_{12}$Sr$_3$Ca$_6$Mn$_3$NbSi$_2$O$_7$O(OH)$_2$O$_4$(OH,Cl)$_2$ [20].

Comparative data for odikhinchaite, other M$_3$Nb- and M$_2$Mn$^{2+}$-dominant eudialyte-group minerals structurally related to odikhinchaite and taseqite are given in Table 6.

Table 6. Comparative data for odikhinchaite and some related eudialyte-group minerals .

| Mineral                   | Odikhinchaite                              | Taseqite                                  | Kentbrook-Site                          | Carbokentbrooksite                      | Zirsklite-(Ce)                |
|---------------------------|--------------------------------------------|-------------------------------------------|-----------------------------------------|----------------------------------------|-----------------------------|
| Formula                   | Na$_{19}$Sr$_3$[(H$_2$O)$_2$Na]Ca$_6$Mn$_3$Zr$_3$NbSi(Si$_2$O$_7$)O(OH)$_3$SiO$_3$H$_2$O | Na$_{12}$Sr$_3$Ca$_2$Fe$^{2+}_2$Zr$_3$NbSi(Si$_2$O$_7$)O(OH)$_3$SiO$_3$H$_2$O | Na$_{12}$Ca$_2$Mn$_3$Zr$_3$NbSi(Si$_2$O$_7$)O(OH)$_3$SiO$_3$H$_2$O | (Na$_2$,RE)$_3$Ca$_6$Mn$_3$Zr$_3$NbSi(Si$_2$O$_7$)O(OH)$_3$SiO$_3$H$_2$O | (Na$_2$,Ce,Na)$_3$Ca$_6$Mn$_3$Zr$_3$NbSi(Si$_2$O$_7$)O(OH)$_3$SiO$_3$H$_2$O |
| N3 site                   |                                           |                                           | Na                                      | Na                                     | Ce$^{3+}$                   |
| M2 site                   | Sr                                        | Sr                                        | Mn$^{2+}$                               | Mn$^{2+}$                              | Mn$^{2+}$                   |
| a, Å                      | 14.2179                                   | 14.2828                                   | 14.1686                                 | 14.239                                 | 14.248                      |
| c, Å                      | 30.349                                    | 30.0222                                   | 30.0847                                 | 30.039                                 | 30.076                      |
| V, Å$^3$                  | 5313.1                                    | 5303.9                                    | 5260                                    | 5274                                   | 5288                        |
| Optical data              | Uniaxial (–)                               | Uniaxial (–)                               | Uniaxial (–)                            | Uniaxial (–)                           | Uniaxial (–)                |
| ω, ε                      | 1.638                                      | 1.649                                     | 1.628                                   | 1.645                                  | 1.648                       |
| Density, g·cm$^{-3}$      | 2.97 (measured)                           | 3.24 (measured)                           | 3.10 (measured)                        | 3.14 (measured)                       | 3.15 (measured)            |

* All the minerals are trigonal, space group R3m, Z = 3.

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