Article

Odikhinchaite, $Na_9Sr_3[(H_2O)_2Na]Ca_6Mn_3Zr_3NbSi$ $(Si_{24}O_{72})O(OH)_3(CO_3) \cdot H_2O$, a New Eudialyte-Group Mineral from the Odikhincha Intrusion, Taimyr Peninsula, Russia

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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 alkaline–carbonatite intrusion, Taimyr Peninsula, Krasnoyarsk Krai, Russia. Associated minerals are orthoclase, albite, aegirine, cancrinite, ancylite-(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(meas.) is 2.97(1) g·cm^{-3}, D(calc.) is 3.04 g·cm^{-3}. Odikhinchaite is optically uniaxial (–), ω = 1.638(2), ε = 1.630(2). The IR spectrum shows the presence of the $^{IV}Mn^{2+}O_4$ polyhedra, H_2O molecules and CO_3^{2-} anions. The chemical composition is (electron microprobe, H_2O determined by the modified Penfield method, CO_2 determined by selection sorption of gaseous annealing products; wt%): Na_2O 9.25, K_2O 0.59, CaO 12.77, MnO 5.49, FeO 0.75, MgO 0.24, La_2O_3 0.38, Ce_2O_3 0.39, Nd_2O_3 0.15, Al_2O_3 0.07, SiO_2 44.80, ZrO_2 11.13, TiO_2 0.07, Nb_2O_5 4.17, Cl 0.69, CO_2 0.90, H_2O 2.22, –O = Cl –0.16, 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): ${^{N1}(Na_{2.58}Ca_{0.42})^{N2}[Na_{2.37}Ca_{0.51}(H_2O)_{0.12}]^{N3}(Sr_{2.00}K_{0.45}Na_{0.35}REE_{0.20})^{N4}Na_3^{N5}[(H_2O)_{1.8}Na_{1.2}]}\{^ZZr_3^{M1}Ca_6^{M2}(Mn_{2.49}Fe^{2+}_{0.51})[^{M3}Nb(OH)_{1.82}O_{1.18}](^{M4}SiOH)[Si_3O_9]_2[Si_9O_{27}]_2^{X1}[(CO_3)_{0.53}Cl_{0.47}]^{X2}[(H_2O)_{0.6}(O,F)_{0.4}]^{XM4}(CO_3)_{0.15}}$. The strongest lines of the powder X-ray diffraction pattern [d, Å (I, %) (hkl)] are: 11.42 (64) (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 $[N1 N2 N3 N4 N5]_3 M1_6 M2_3 M3 M4 Z_3 (Si_9 O_{27})_2 (Si_3 O_9)_2 Ø_{4-6} X1 X2$, where Z = Zr, Ti, Nb; $M1$ = Ca, Mn^{2+}, Fe^{2+}, Na, *REE*; $M2$ = Fe^{2+}, Fe^{3+}, Mn^{2+}, Zr, Na; $M3–4$ = Si, Nb, W; $N1–5$ = Na, Ca, Mn, Sr, K, *REE*, H_2O, H_3O; $Ø$ = OH; X = Cl, H_2O, CO_3. The eudialyte-type crystal structure is based on a heteropolyhedral pseudo-framework built up by the rings of tetrahedra (Si_3O_9 and Si_9O_{27}) and of octahedra ($M1_6O_{24}$) connected via $M2O_{4-7}$ polyhedra and ZO_6 octahedra containing additional $M3$ and $M4$ sites, which are situated at the centers of two nonequivalent Si_9O_{27} rings and can be filled by additional $TØ_4$-tetrahedra (predominantly occupied by silicon) or ($MØ_6$)-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_2O 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^-, S^{2-}, SO_4^{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 ^{N3}Sr, $^{N5}(H_2O)$, $^{M2}Mn^{2+}$, ^{M3}Nb, and $^{X1}(CO_3^{2-})$ 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 Anabarskiy 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 turjaites) 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 poikilite-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 1×0.5 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: $Na_{12.3–12.4}K_{0.5}Ca_{6–6.4}Sr_{1.5–1.7}Fe_{1.9–2.4}Mn_{0.5–0.7}Nb_{0.5–0.6}Ti_{0.2–0.5}Zr_{2.5–2.7}Si_{25.3–25.5}O_{73}(O,H_2O,Cl)_5$ [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_2O 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), Co$K\alpha$, 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.

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.

(**a**)	(**b**)
(**c**)	(**d**)
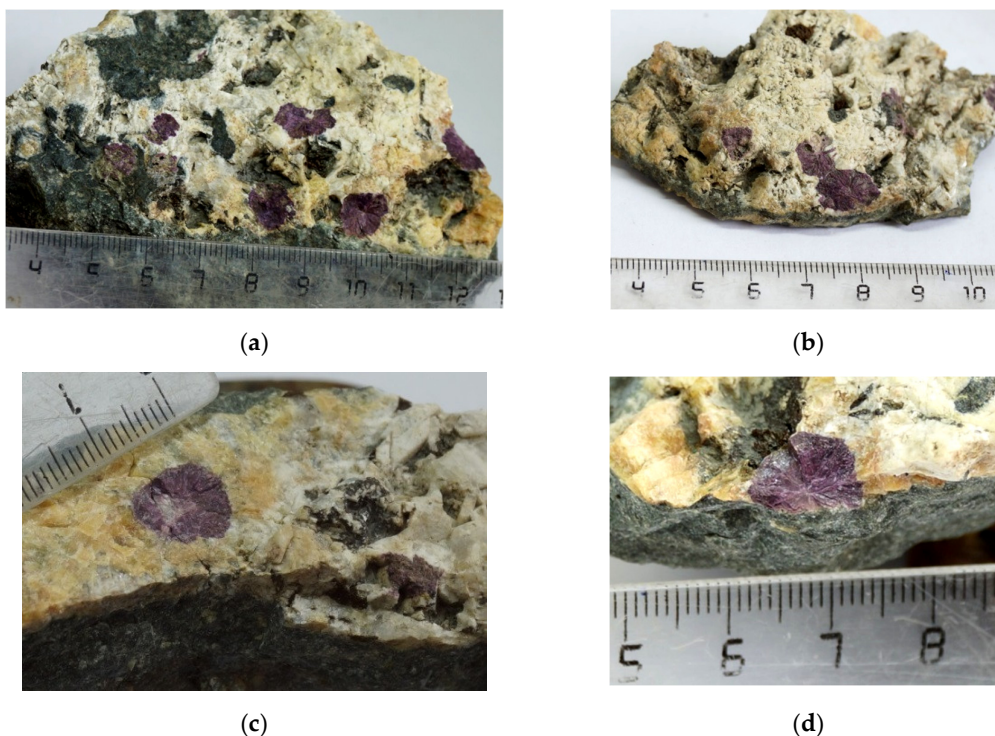
Figure 1. Odikhinchaite aggregates (purple rosettes) in pegmatite with white alkali feldspars, yellow cancrinite and dark green to black aegirine.

Table 1. Crystal data, data collection information and structure refinement details for odikhinchaite.

Crystal Data	
Simplified formula	$Na_9Sr_3[(H_2O)_2Na]Ca_6Mn_3Zr_3NbSi(Si_{24}O_{72})O(OH)_3(CO_3)\cdot H_2O$
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; λ	Mo*K*α; 0.71073
Absorption coefficient, μ (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_{min}, T_{max}	0.773; 1
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	27,254, 2345, 2312
R_{int}	0.053
$(\sin\theta/\lambda)_{max}$ (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_{par})	265
N_{ref}/N_{par}	8.73
ΔQ_{max}, ΔQ_{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 (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].

(**a**)

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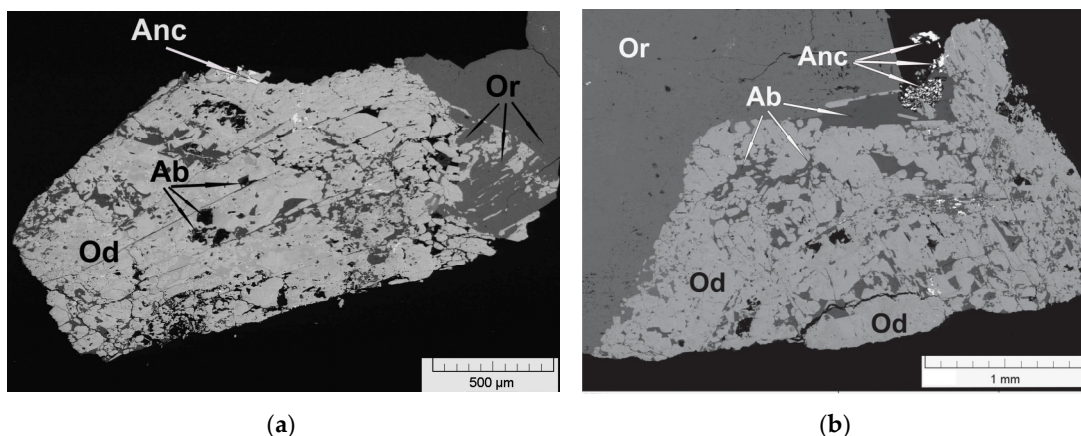
Figure 2. Fragments of odikhinchaite (Od) individuals with albite (Ab) inclusions in association with ancylite-(Ce) (Anc) and orthoclase (Or). BSE images of polished sections.

The IR spectrum of odikhinchaite differs from that of its $^{M2}Fe^{2+}$-dominant and CO_2-deficient analogue taseqite with the crystal-chemical formula $[Na_{10.5}K_{0.5}(Sr_{1.71}Na_{1.29})][Ca_{5.85}REE_{0.15}][Zr_{2.96}Hf_{0.03}](Fe^{2+}_{2.43}Mn_{0.45})Si(Nb_{0.64}Ti_{0.27})(Si_9O_{27})_2(Si_3O_9)_2(OH,O,Cl)_5$

from the Odikhincha massif (curve *b* on Figure 3) in higher intensities of the bands of O–H, C–O, Nb–O and $^{IV}Mn^{2+}$–O stretching vibrations and a lower intensity of the band of $^{IV}Fe^{2+}$–O stretching vibrations, which is in accordance with crystal-chemical features of these minerals.
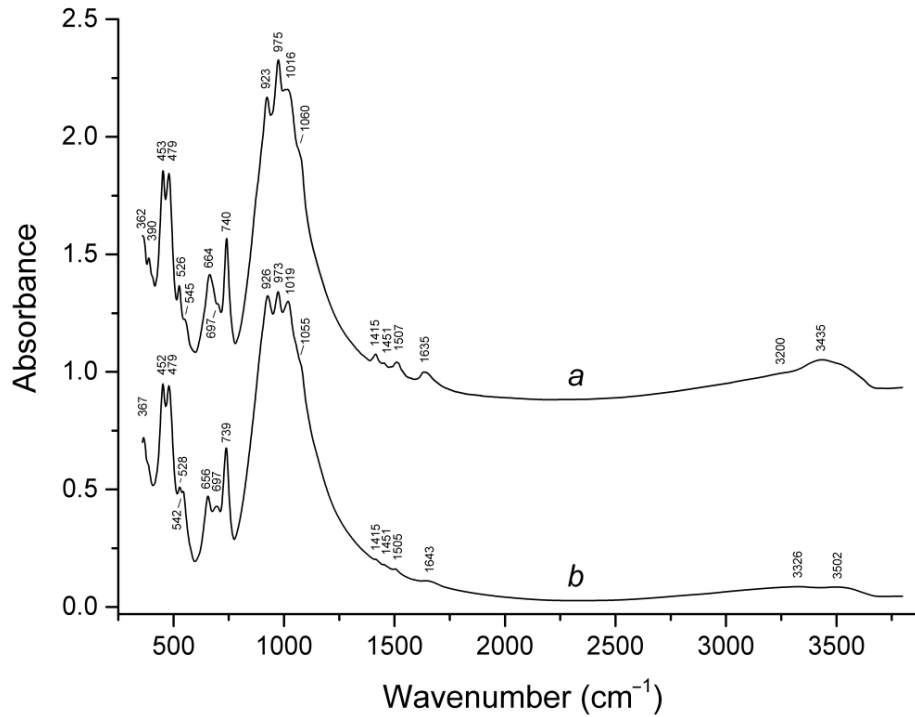
Figure 3. Powder infrared absorption spectra of (**a**) odikhinchaite and (**b**) taseqite, both from the Odikhincha alkaline complex.

4.3. Optical Properties

Odikhinchaite is optically uniaxial (–), ω = 1.638(2), ε = 1.630(2) (λ = 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.

Table 2. Chemical data for odikhinchaite.

Constituent	Mean Content, wt%	Range	Standard Deviation	Probe Standard
Na_2O	9.26	8.97–9.68	0.29	Albite
K_2O	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	SrF_2
La_2O_3	0.38	0.11–0.63	0.12	$LaPO_4$
Ce_2O_3	0.39	0–1.41	0.15	$CePO_4$

Nd$_2$O$_3$	0.15	0–0.42	0.21	NdPO$_4$
Al$_2$O$_3$	0.07	0–0.17	0.11	Albite
SiO$_2$	44.80	44.12–45.74	0.74	SiO$_2$
ZrO$_2$	11.13	10.82–11.72	0.19	Zr
TiO$_2$	0.07	0–0.41	0.14	Ti
Nb$_2$O$_5$	4.17	3.21–4.74	0.21	Nb
Cl	0.69	0.61–0.83	0.02	NaCl
CO$_2$	0.90	-	-	-
H$_2$O	2.22	-	-	-
–O = Cl	–0.16	-	-	-
Total	99.72	-	-	-

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 $H_{8.22}Na_{9.97}K_{0.42}Ca_{7.59}Sr_{1.87}Ce_{0.08}La_{0.08}Nd_{0.03}Mn_{2.58}Fe_{0.35}Mg_{0.20}Ti_{0.03}Zr_{3.01}Nb_{1.05}Si_{24.87}Al_{0.05}Cl_{0.65}C_{0.68}O_{81.71}$.

The end-member formula is $Na_9Sr_3[(H_2O)_2Na]Ca_6Mn_3Zr_3NbSi(Si_{24}O_{73})(OH)_3(CO_3)·H_2O$.

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.

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 *R*3*m*. The unit-cell parameters calculated from the powder data are: *a* = 14.2179(1), *c* = 30.3492(3) Å, *V* = 5313.1(1) Å^3.

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

I_{obs}	d_{obs}	I_{calc} *	d_{calc} **	h k l	I_{obs}	d_{obs}	I_{calc} *	d_{calc} **	h k l
64	11.42	100	11.439	101	17	2.138	4	2.144	057
							4	2.141	0.3.12
							8	2.138	3.1.11
							8	2.131	514
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
								2.062	600
24	6.05	22	6.058	021	8	2.055	5	2.053	247
							2	2.051	2.2.12
							1	2.048	0.4.11
39	5.71	26	5.720	202	4	2.027	5	2.029	431
3	5.42	1	5.409	015	6	2.019	5	2.019	603
							3	2.015	342
6	5.01	6	5.012	006	19	1.984	17	1.985	428
							3	1.981	520
3	4.774	2	4.776	024	3	1.952	4	1.952	1.2.14
3	4.611	3	4.620	211	9	1.938	2	1.943	253
							9	1.939	339
41	4.309	22	4.312	205	6	1.918	5	1.918	1.3.13
							1	1.913	158
19	4.100	13	4.102	116	13	1.907	1	1.910	0.5.10
							12	1.907	606
25	3.967	22	3.970	214	3	1.881	2	1.883	161
19	3.810	11	3.813	303	3	1.872	2	1.872	612
7	3.689	7	3.691	125	4	1.856	2	1.858	1.0.16
							1	1.852	4.0.13
28	3.567	7	3.596	018	20	1.839	5	1.846	2.4.10
		19	3.571	220			9	1.842	526
							5	1.838	437

I	d	I	d	hkl	I	d	I	d	hkl
							6	1.836	1.4.12
30	3.529	19	3.528	027	8	1.798	3	1.803	0.3.15
							4	1.800	615
							2	1.798	0.2.16
							2	1.793	3.2.13
53	3.405	46	3.409	131	27	1.785	2	1.788	348
							4	1.787	5.1.10
							22	1.785	440
							4	1.777	4.2.11
15	3.344	9	3.345	312	13	1.764	13	1.764	701
		1	3.341	009					
45	3.208	37	3.212	208	6	1.749	1	1.755	072
		23	3.184	036			1	1.755	609
							4	1.748	2.2.15
44	3.167	36	3.163	217	7	1.722	1	1.727	167
							3	1.726	3.3.12
							6	1.720	704
3	3.121	6	3.121	134	8	1.713	5	1.713	621
31	3.025	12	3.029	042	7	1.704	5	1.704	262
		16	3.026	119			1	1.704	259
							1	1.701	2.0.17
100	2.978	91	2.980	315	12	1.682	1	1.686	618
							4	1.685	4.3.10
							9	1.682	446
21	2.908	18	2.908	226	2	1.670	1	1.671	0.0.18
86	2.858	74	2.860	404	10	1.647	5	1.650	265
							3	1.648	1.3.16
							4	1.644	2.4.13
5	2.787	7	2.789	232	5	1.627	2	1.631	3.4.11
							4	1.627	1.1.18
							1	1.622	5.0.14
3	2.747	4	2.750	045	14	1.606	2	1.609	4.1.15
							13	1.606	4.0.16
19	2.699	11	2.704	0.2.10	10	1.596	3	1.599	538
		7	2.699	410			6	1.598	1.6.10
		8	2.681	137			4	1.593	627
							1	1.592	0.6.12
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	3.2.16
		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	2.5.12
							1	1.553	6.1.11
							3	1.550	544
7	2.508	5	2.510	407	8	1.546	1	1.548	0.3.18
		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	4.3.13
							1	1.524	3.5.10
5	2.439	1	2.441	502	1	1.513	1	1.514	084
		3	2.440	229			1	1.513	2.2.18
19	2.378	5	2.388	048	3	1.497	2	1.497	0.5.16
		9	2.380	330			1	1.493	0.1.20
		9	2.377	416					
13	2.329	13	2.331	241	11	1.484	2	1.486	547
							8	1.484	0.7.11
							2	1.482	274
							4	1.477	3.4.14
6	2.264	3	2.265	238	5	1.465	2	1.466	725
		2	2.261	1.3.10			3	1.465	2.4.16
							2	1.460	458

3	2.213	4	2.216	511	2	1.454	1	1.454	4.4.12
							1	1.453	2.6.11
7	2.196	7	2.198	152	5	1.437	3	1.437	0.6.15
							1	1.437	1.3.19
							1	1.435	5.1.16
6	2.178	5	2.179	425	9	1.430	1	1.432	0.0.21
							2	1.431	1.2.20
							1	1.430	808
							5	1.428	550
							1	1.426	277
16	2.154	10	2.156	4.0.10	5	1.417	1	1.420	4.1.18
		2	2.150	336			5	1.417	461
							2	1.413	642

* For the calculated pattern, only reflections with intensities ≥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, Å^2), site multiplicities (*Mult*), site occupancies and bond-valence sums (BVS) in the structure of odikhinchaite.

Site	x	y	z	U_{iso}*/U_{eq}	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)$_{0.607}$O$_{0.393}$	-
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)$_{0.82}$	-

*M*4b	0	0	0.9192(7)	0.026(6)	3	$Si_{0.18}$	-
OH^{M4b}	0	0	0.975(2)	0.0612(6) *	3	$(OH)_{0.18}$	-
*N*1	0.4366(2)	0.5634(5)	0.1300(1)	0.0299(9)	9	$Na_{0.79}Ca_{0.17}(H_2O)_{0.04}$	-
*N*2a	−0.1093(3)	0.1093(3)	0.1525(2)	0.0415(17)	9	$Na_{0.86}$	-
*N*2b	−0.0782(7)	0.0782(7)	0.1343(6)	0.033(4)	9	$Ca_{0.14}$	-
*N*3a	0.23412(1)	0.46830(7)	0.25630(4)	0.0167(2)	9	$Sr_{0.667}K_{0.15}Ln_{0.067}$	-
*N*3b	0.2357(14)	0.471(3)	0.2267(12)	0.031(7) *	9	$Na_{0.116}$	-
*N*4	0.1018(4)	0.2036(8)	0.0182(2)	0.084(5)	9	Na	-
*N*5	−0.2630(2)	0.2630(2)	0.1180(2)	0.037(2)	9	$(H_2O)_{0.6}Na_{0.4}$	-
*X*1a	1/3	2/3	0.2027(3)	0.0237(17)	3	$C_{0.53}Cl_{0.35}$	-
OC^{X1a}	0.3827(3)	0.6173(3)	0.2125(8)	0.091(8) *	9	$O_{0.53}$	-
*X*1b	1/3	2/3	0.1541(13)	0.039(7) *	3	$Cl_{0.12}$	-
*X*2a	0	0	0.0556(12)	0.056(10)	3	$(H_2O)_{0.6}$	-
*X*2b	0	0	0.0898(18)	0.064(12) *	3	$(OH,F)_{0.4}$	-
C^{XM4}	0	0	0.997(8)	0.057(12) *	3	$C_{0.15}$	-
OC^{XM4}	−0.0509(2)	0.0509(2)	0.999(3)	0.08(2) *	3	$O_{0.15}$	-

Note: *U_{iso}; Bond-valence sums were calculated using the bond-valence parameters for the Zr^{4+}–O, Mn^{2+}–O, Fe^{2+}–O, and Nb^{5+}–O bonds [16], as well as Si^{4+}–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
	O4	2.050(6)		O14	2.484(6)
	O2 × 2	2.074(5)		O8	2.500(7)
Z	O16 × 2	2.086(4)		O4	2.639(7)
	O10	2.093(5)		O4	2.641(4)
	-	2.077	*N*1	O16 × 2	2.652(4)
	O17	2.287(5)		X1b	2.655(11)
	O3	2.332(5)		OC^{X1a}	2.816(22)
	O5	2.348(5)		O13 × 2	2.823(5)
*M*1	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)
	O3	1.601(5)	*N*2a	O15	2.671(8)
	O10	1.605(6)		O1	2.683(7)
Si1	O15 × 2	1.651(4)		O9 × 2	2.802(7)
	-	1.627		-	2.651
	O12	1.598(5)		N1b	0.945(16)
	O6	1.606(5)		X2b	2.352(34)
Si2	O13	1.663(5)		O2 × 2	2.385(11)
	O13	1.663(4)		O10	2.427(12)
	-	1.633	*N*2b	O10	2.428(12)
	O11	1.599(4)		O1	2.938(15)
	O2	1.603(5)		O15	2.973(19)
Si3	O13	1.645(5)		X2a	3.057(32)
	O1	1.665(3)		-	2.618
	-	1.628		OC^{X1a} × 2	2.500(13)
	O17	1.565(6)		O7 × 2	2.542(4)
	O4	1.602(6)		O12	2.639(5)
Si4	O8	1.647(5)		OH^{M3} × 2	2.681(5)
	O8	1.648(6)	*N*3a	O16 × 2	2.854(5)
	-	1.616		O3	2.891(5)
	O18	1.582(7)		X1a	2.936(5)
	O5	1.587(6)		-	2.693
Si5	O9	1.633(6)		N3b	0.891(36)
	O9	1.633(5)		OC^{X1a}	2.138(25)
	-	1.609	*N*3b	OC^{X1a}	2.141(44)
Si6	O16	1.588(5)		O16	2.206(34)

	Atom	Value		Atom	Value
	O7	1.608(4)		O16	2.210(27)
	O9	1.627(5)		X1a	2.526(37)
	O14	1.635(3)		O7	2.732(37)
	-	1.615		O7	2.737(24)
	-	-		-	2.384
M2	OH^{M3}	2.105(4)		OC^{XM4} × 2	2.256(24)
	O7 × 2	2.106(4)		O11 × 2	2.574(11)
	O11 × 2	2.113(4)		O5	2.597(9)
	-	2.109	N4	X2a	2.758(17)
M3	OH^{M3} × 3	1.891(4)		OH^{M4b}	2.835(9)
	O6 × 3	2.081(6)		O2 × 2	2.878(9)
	-	1.986		O17	3.010(12)
M4a	OH^{M4a}	1.598(13)		-	2.662
	O18 × 3	1.630(4)		OH^{M4a}	2.217(9)
	-	1.622		O1	2.241(6)
	M4b	1.076(22)	N5	O6 × 2	2.503(6)
M4b	OH18 × 3	1.547(8)		N5 × 2	3.014(5)
	O^{M4b}	1.675(21)		O13 × 2	3.072(5)
	-	1.579		-	2.705
X1a	OC^{X1a} × 3	1.256(7)	X^{M4}	OC^{XM4} × 3	1.260(5)
	X1b	1.461(40)		OH^{M4b}	0.676(12)

Odikhinchaite is isostructural with other 12-layered members of the eudialyte group with the space group *R*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):

$\{^{N1}(\mathrm{Na}_{2.58}\mathrm{Ca}_{0.42})^{N2}[\mathrm{Na}_{2.37}\mathrm{Ca}_{0.51}(\mathrm{H_2O})_{0.12}]^{N3}(\mathrm{Sr}_{2.00}\mathrm{K}_{0.45}\mathrm{Na}_{0.35}REE_{0.20})^{N4}\mathrm{Na}_3{}^{N5}[(\mathrm{H_2O})_{1.8}\mathrm{Na}_{1.2}]\}\{^{Z}\mathrm{Zr}_3{}^{M1}\mathrm{Ca}_6{}^{M2}(\mathrm{Mn}_{2.49}\mathrm{Fe}^{2+}{}_{0.51})[^{M3}\mathrm{Nb}(\mathrm{OH})_{1.82}\mathrm{O}_{1.18}](^{M4}\mathrm{SiOH})[\mathrm{Si}_3\mathrm{O}_9]_2[\mathrm{Si}_9\mathrm{O}_{27}]_2{}^{X1}[(\mathrm{CO}_3)_{0.53}\mathrm{Cl}_{0.47}]^{X2}[(\mathrm{H_2O})_{0.6}(\mathrm{O,F})_{0.4}]^{XM4}(\mathrm{CO}_3)_{0.15}$
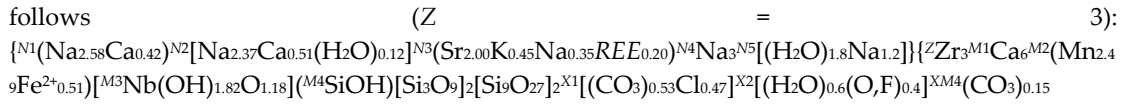
where braces and brackets enclose contents of the key sites.
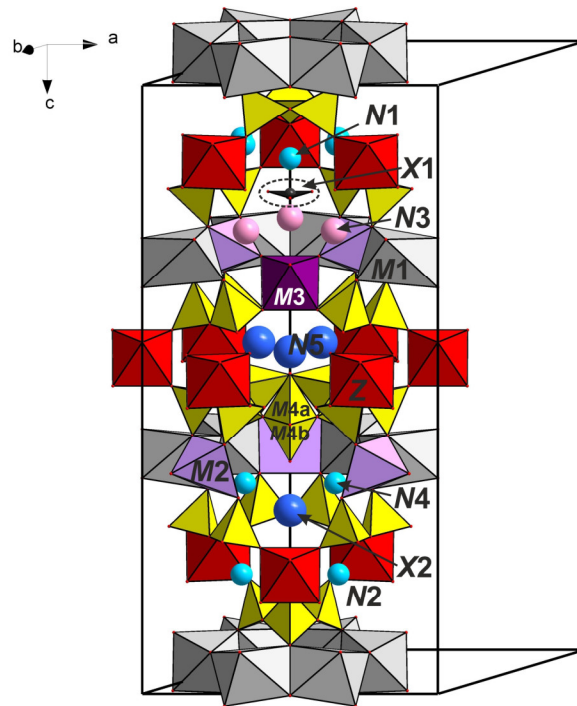
Figure 4. The general view of the crystal structure of odikhinchaite (the unit cell is outlined).
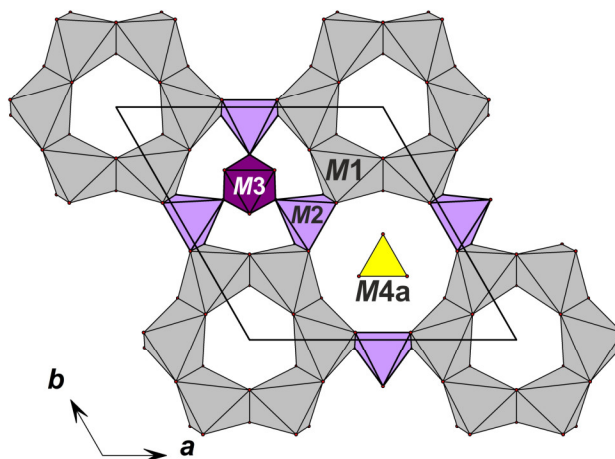
Figure 5. Heteropolyhedral layer involving rings of CaO_6 octahedra in the structure of odikhinchaite.

In the crystal structure of odikhinchaite, manganese (2.49 *apfu*) predominates over iron(II) (0.51 *apfu*) at the *M*2-site, which is located in the center of the $M2\varphi_5$-square pyramids ($\varphi = O^{2-}$, OH^-) with the mean distance $<M2–\varphi> = 2.109$ Å. The octahedral *M*3 site (the mean distance $<M3–\varphi> = 1.986$ Å) located on the threefold axis at the center of one nine-membered Si_9O_{27}-tetrahedral ring is occupied by niobium (1 *apfu*) while the *M*4 site located at the center of the symmetrically non-equivalent nine-membered tetrahedral ring is split into two *M*4a- and *M*4b-sites (*M*4a–*M*4b = 1.076 Å) occupied by silicon (0.82 and 0.18 *apfu*, respectively) in tetrahedral environment (the mean distances are: $<M4a–\varphi> = 1.622$ Å; $<M4b–\varphi> = 1.579$ Å). The $M3\varphi_6$ octahedron links with the $M2\varphi_6$ square pyramid via the common OH^{M3}-vertex forming a heteropolyhedral $[NbMn_3(OH,O)_3]$ cluster (Figure 6).

The distribution of large cations over the *N*1–5 sites in odikhinchaite is similar to that in taseqite [16] and its Cl-deficient variety [10]. The *N*1 site is split into two sites with the distance *N*1a–*N*1b = 0.945 Å. The *N*1a is occupied by sodium (2.58 *apfu*), while *N*1b is occupied by calcium (0.42 *apfu*). The *N*2 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 *N*4 site is fully occupied by sodium. The *N*5 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 *N*3 site. In the structure of odikhinchaite, the *N*3 is split into two sites with the distance *N*3a–*N*3b = 0.891 Å. The *N*3a 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 *X*1a site contains Cl^- or CO_3^{2-}, respectively) (Figure 6a). The *N*3b 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 *X*1 site, which is split into two sites with the distance *X*1a–*X*1b = 1.461 Å. The *X*1a is occupied by CO_3^{2-} (0.53 anions *pfu*) with admixture of chlorine (0.35 *apfu*), while the *X*1b site is occupied only by chlorine (0.12 *apfu*). The *X*2 site is also split into two sites with the distance *X*2a–*X*2b = 1.028 Å. The *X*2a site is occupied by water molecules (0.6 *apfu*) and the *X*2b 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 *X*2a and OH^{M4b} sites with the distances X^{M4}–*X*2a = 1.762 Å and X^{M4}–OH^{M4a} = 0.662 Å.
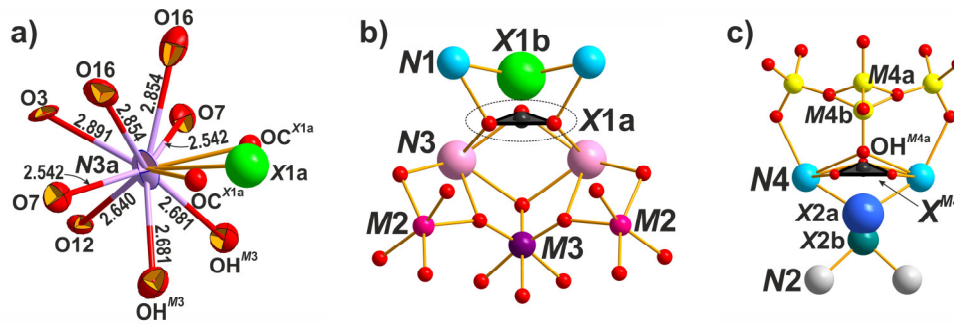
Figure 6. Local coordinational environments of the *N*3a site (**a**), the *X*1 site (**b**), and the *X*2 site (**c**).

5. Discussion

Odikhinchaite Na$_9$Sr$_3$[(H$_2$O)$_2$Na]Ca$_6$Mn$_3$Zr$_3$NbSi(Si$_{24}$O$_{72}$)O(OH)$_3$(CO$_3$)·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$_6$Fe^{2+}$_3$Zr$_3$NbSi(Si$_{24}$O$_{72}$)(O,OH,H$_2$O)$_4$Cl$_2$ [18]. Unlike taseqite, which is Fe^{2+}-dominant at the *M*2 site, in odikhinchaite, this site is predominantly populated by Mn^{2+}. In addition, in odikhinchaite, the *X*2 site is predominantly occupied by the CO$_3$$^{2-}$ groups, whereas in taseqite, this site is Cl-dominant, and the *N*5 site of odikhinchaite is predominantly populated by H$_2$O.

Odikhinchaite can also be the [^{N3}Sr, ^{N5}(H$_2$O)] analogue of carbokentbrooksite (Na,□,*REE*)$_{15}$Ca$_6$Mn$_3$Zr$_3$NbSi(Si$_{24}$O$_{72}$)O(OH)$_3$(CO$_3$)·H$_2$O [19] and the [^{M3}Nb, ^{N5}(H$_2$O), ^{X1}(CO$_3$)] analogue of manganokhomyakovite Na$_{12}$Sr$_3$Ca$_6$Mn$_3$Zr$_3$WSi(Si$_{24}$O$_{72}$)(O,OH,H$_2$O)$_4$(OH,Cl)$_2$ [20].

Comparative data for odikhinchaite, other ^{M3}Nb- and ^{M2}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	Carbokent-Brooksite	Zirsilite-(Ce)
Formula	Na$_9$Sr$_3$[(H$_2$O)$_2$Na] Ca$_6$Mn$_3$Zr$_3$NbSi (Si$_{24}$O$_{72}$)O(OH)$_3$ (CO$_3$)·H$_2$O	Na$_{12}$Sr$_3$Ca$_6$Fe^{2+}$_3$ Zr$_3$NbSi(Si$_{24}$O$_{72}$) (O,OH,H$_2$O)$_4$Cl$_2$	Na$_{15}$Ca$_6$Mn$_3$ Zr$_3$NbSi (Si$_{24}$O$_{72}$)O$_2$ F$_2$·2H$_2$O	(Na,□,*REE*)$_{15}$Ca$_6$ Mn$_3$Zr$_3$NbSi (Si$_{24}$O$_{72}$)O(OH)$_3$ (CO$_3$)·H$_2$O	(Na,□)$_{12}$(Ce,Na)$_3$ Ca$_6$Mn$_3$Zr$_3$Nb Si(Si$_{24}$O$_{72}$)O (OH)$_3$(CO$_3$)·H$_2$O
*N*3 site	Sr	Sr	Na	Na	Ce^{3+}
*M*2 site	Mn^{2+}	Fe^{2+}	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 (−) ω = 1.638 ε = 1.630	Uniaxial (−) ω = 1.6494 ε = 1.6378	Uniaxial (−) ω = 1.628 ε = 1.623	Uniaxial (−) ω = 1.645 ε = 1.635	Uniaxial (−) ω = 1.648 ε = 1.637
Density, g·cm^{-3}	2.97 (measured) 3.04 (calculated)	3.24 (measured) 3.20 (calculated)	3.10 (measured) 3.08 (calculated)	3.14 (measured) 3.10 (calculated)	3.15 (measured) 3.10 (calculated)

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

Author Contributions: N.V.C., Y.D.G. and S.M.A. wrote the paper. Y.D.G. collected the type material. D.A.K. obtained single-crystal X-ray diffraction data. S.M.A. solved and refined the crystal structure. S.N.B. and I.V.P. obtained and treated powder X-ray diffraction data. D.A.V. conceived and designed chemical data. N.V.C. obtained IR spectra. L.A.P. obtained optical data and measured hardness. S.A.V. measured density. All authors have read and agreed to the published version of the manuscript.

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