НОВЫЕ МИНЕРАЛЫ

NIOBOIXIOLITE-(Mn^{2+}), $\left(Nb_{2/3}Mn^{2+}_{1/3}\right)O_2$, A NEW IXIOLITE-GROUP MINERAL FROM THE MALKHAN PEGMATITE FIELD, TRANSBAIKAL REGION, RUSSIA

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The new ixiolte-group mineral nioboixiolite-(Mn^{2+}), ideally $\left(Nb_{2/3}Mn^{2+}_{1/3}\right)O_2$, the niobian analogue of ixiolite-(Mn^{2+}), was discovered in the Sosedka granitic pegmatite vein, Malkhan pegmatite field, Zabaikalsky Krai (Transbaikal Region), Siberia, Russia. The associated minerals are albite, quartz, microcline, elbaite, beryl, bismuthinite, euxenite-(Y), zircon, rutile, cassiterite, and cannonite. Nioboixiolite-(Mn^{2+}) occurs as clusters of dark brown to brown-black prismatic crystals up to 0.8 × 1.5 × 5 mm embedded in albite. The lustre is submetallic to adamantine, and the streak is brown. Cleavage is not observed. The Mohs' hardness is 4.5–5. Density calculated using the empirical formula is equal to 5.803 g cm^{-3}. The IR spectrum and reflectance spectra in visible range are given. The chemical composition of nioboixiolite-(Mn^{2+}) is (electron microprobe, wt %): MnO 14.94, Sc_2O_3 1.80, Fe_2O_3 0.20, Y_2O_3 1.34, TiO_2 7.66, ZrO_2 1.74, SnO_2 1.01, ThO_2 0.26, UO_2 1.44, Nb_2O_5 42.80, Ta_2O_5 26.77, total 99.96. The empirical formula is $(Nb_{1.59}Mn^{2+}_{1.04}Ta_{0.59}Ti_{0.47}Sc_{0.13}Zr_{0.07}Y_{0.06}Sn_{0.03}U_{0.03}Fe^{3+}_{0.01})_{\Sigma 4.02}O_8$ (Z = 1). The crystal structure was determined using single-crystal X-ray diffraction data and refined to R = 0.0474. The new mineral is isostructural to other ixiolite-group members. Nioboixiolite-(Mn^{2+}) is orthorhombic, space group: *Pbcn*, a = 4.762(2) Å, b = 5.739(1) Å, c = 5.149(1) Å, V = 140.7(1) $Å^3$. The strongest lines of the powder X-ray diffraction pattern [d, Å (I, %) (*hkl*)] are: 3.662 (29) (110), 2.984 (100) (111), 2.505 (21) (021), 1.775 (21) (130), 1.748 (28) (202), 1.726 (35) (221), 1.553 (20) (113), 1.473 (19) (023), 1.463 (30) (311, 132).

Keywords: nioboixiolite-(Mn^{2+}), new mineral, ixiolite group, columbite supergroup, crystal structure, Malkhan pegmatite field

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1. INTRODUCTION

According to the recently approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA CNMNC) nomenclature of columbite-supergroup minerals (IMA MEMORANDUM 108-SM22; Chukanov et al., 2022), the well-known mineral ixiolite got the new species name ixiolite-(Mn^{2+}) and the ide-

alized formula $\left(Ta_{2/3}Mn^{2+}_{1/3}\right)O_2$. The new mineral species nioboixiolite-(Mn^{2+}), ideally $\left(Nb_{2/3}Mn^{2+}_{1/3}\right)O_2$, described in this paper is isostructural with ixiolite-(Mn^{2+}) being its Nb-dominant analogue. Nioboixiolite-(Mn^{2+}) is also isostructural with other members of the ixiolite group, scrutinyite α-PbO_2 (Zaslavskiy and Tolkachev, 1952; Taggart et al., 1988), srilankite, $(Ti,Zr)O_2$ (Willgallis et al., 1983; Willgalis and Hartl, 1983), and seifertite, SiO_2 (Dera et al., 2002; El Goresy et al., 2008; Zhang et al., 2016). Thus, nioboixiolite-(Mn^{2+}) is a niobium analogue of all these minerals belonging to the α-PbO_2 structure type.

The new mineral nioboixiolite-(Mn^{2+}) and its name were approved by the IMA CNMNC (IMA No. 2021-050a). The type specimen is deposited in the collections of the Fersman Mineralogical Museum of the Russian Academy of Sciences, Moscow, Russia, with registration number 5721/1.

2. EXPERIMENTAL METHODS

Fourteen electron microprobe analyses were carried out using a Jeol JSM-6480LV scanning electron microscope equipped with an INCA-Wave 500 wavelength-dispersive spectrometer (Laboratory of Analytical Techniques of High Spatial Resolution, Dept. of Petrology, Moscow State University), with an acceleration voltage of 20 kV, a beam current of 20 nA, and a 3 μm beam diameter.

In order to obtain infrared (IR) absorption spectrum, powdered nioboixiolite-(Mn^{2+}) sample has been mixed with dried KBr, pelletized, and analyzed using an ALPHA FTIR spectrometer (Bruker Optics) in the range of 360–3800 cm^{-1} with a resolution of 4 cm^{-1}. A total of 16 scans were collected. IR spectrum of an analogous pellet of pure KBr was used as a reference.

The reflectance values were measured in air by means of the MSF-21 microspectrophotometer (LOMO, Russia) with SiC (Reflexionsstandard 474251, No. 545, Germany) as a reference material.

Powder X-ray diffraction data were collected using a Rigaku R-AXIS Rapid II diffractometer (image plate), Co$K\alpha$, 40 kV, 15 mA, rotating anode with the microfocus optics, Debye-Scherrer geometry, $r = 127.4$ mm, exposure 15 min. The raw powder XRD data were collected using program suite designed by Britvin et al. (2017). 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 studies were carried out using an Xcalibur diffractometer equipped with a CCD-detector (Mo$K\alpha$ radiation). Crystal data, data collection information and structure refinement details are given in Table 1.

3. RESULTS

3.1. Occurrence, general appearance and physical properties. The holotype specimen of nioboixiolite-(Mn^{2+}) was collected from the Sosedka granitic pegmatite vein, Malkhan pegmatite field, Krasnochikoisky District, Zabaikalsky Krai, Siberia, Russia. The new mineral forms prismatic, typically lath-like crystals up to 0.8 × 1.5 × 5 mm, elongated along [001] and flattened on [100]. They are commonly crude, divergent and sometimes combined in radiating clusters up to 4 mm × 1 cm embedded in albite (Fig. 1). The other associated minerals are quartz, microcline, elbaite, beryl, bismuthinite, euxenite-(Y), zircon, rutile, cassiterite, and secondary cannonite.

Nioboixiolite-(Mn^{2+}) is dark brown to brown-black, the lustre is submetallic on crystal faces and adamantine on the broken surface. The streak is brown. Cleavage is not observed. The fracture is conchoidal. The mean VHN hardness determined by micro-indentation at load of 100 g is equal to 303 kg/mm^2 (range 282–330 kg/mm^2, $n = 5$). The Mohs' hardness is 4.5–5.

Table 1. Data of the single-crystal X-ray diffraction experiment and crystal structure refinement for nioboixiolite-(Mn^{2+})
Таблица 1. Данные монокристального рентгенодифракционного эксперимента и уточнения кристаллической структуры ниобоиксиолита-(Mn^{2+})

Crystal system, space group, Z	Orthorhombic, *Pbcn*, 4
Unit-cell dimensions, Å	$a = 4.7559(5)$ $b = 5.7318(5)$ $c = 5.1344(4)$
V, Å^3	139.97(2)
Crystal size, mm	0.06 × 0.12 × 0.42
Temperature, K	293(2)
Radiation and wavelength, Å	Mo$K\alpha$; 0.71073
Diffractometer	Xcalibur S CCD
Absorption correction	Gaussian
θ range for data collection, °	5.572–28.280
Reflections collected	1684
Independent reflections	174 ($R_{int} = 0.0608$)
Independent reflections with $I > 2\sigma(I)$	149
Refinement method	Full-matrix least-squares on F^2
Number of refined parameters	16
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0474$, w$R2 = 0.0957$
R indices (all data)	$R1 = 0.0592$, w$R2 = 0.1008$
GoF	1.377
Largest diff. peak and hole, e/Å^3	1.96 and –0.80

Density calculated using the empirical formula and unit-cell parameters obtained from single-crystal X-ray diffraction data is equal to 5.803 g cm^{-3}.

Under the microscope in reflected light, nioboixiolite-(Mn^{2+}) is gray, with strong yellowish-brown internal reflections. Bireflectance is weak, $\Delta R = 0.7\%$ (589 nm). Anisotropism is weak. Pleochroism is not observed. Reflectance values are given in Table 2 (the reference wavelengths required by the Commission on Ore Mineralogy are given in bold type).

The IR spectrum of nioboixiolite-(Mn^{2+}) (Fig. 2) is close to that of ixiolite-(Mn^{2+}) (Chukanov, 2014). IR absorption in the range of 400–700 cm^{-1} and below 400 cm^{-1} is due to stretching and bending vibrations of the MO_2 octahedral pseudo-framework (M = Nb, Mn^{2+}, Ta, Ti, etc.). Taking into account that Mn^{2+} is the main low field-strength cation in nioboixiolite-(Mn^{2+}), the band at 480 cm^{-1} may be tentatively assigned to stretching vibrations of the Nb–O–Mn^{2+} fragment. The shoulder at 870 cm^{-1} and the weak band at 1100 cm^{-1} correspond to combination modes. The absence of absorption bands above 1200 cm^{-1} indicates the absence of H-, B- and C-bearing groups. The IR absorption bands of nioboixiolite-(Mn^{2+}) are broad and poor-resolved which indicates disordering of cations, in agreement with the structural data (see below).

3.2. Chemical composition. Analytical data for nioboixiolite-(Mn^{2+}) based on 14 spot analyses of a polished section are given in Table 3. Contents of other elements with atomic numbers higher than that of carbon are below detection limits. H_2O was not measured because no bands corresponding to H-bearing groups are observed in the IR spectrum.

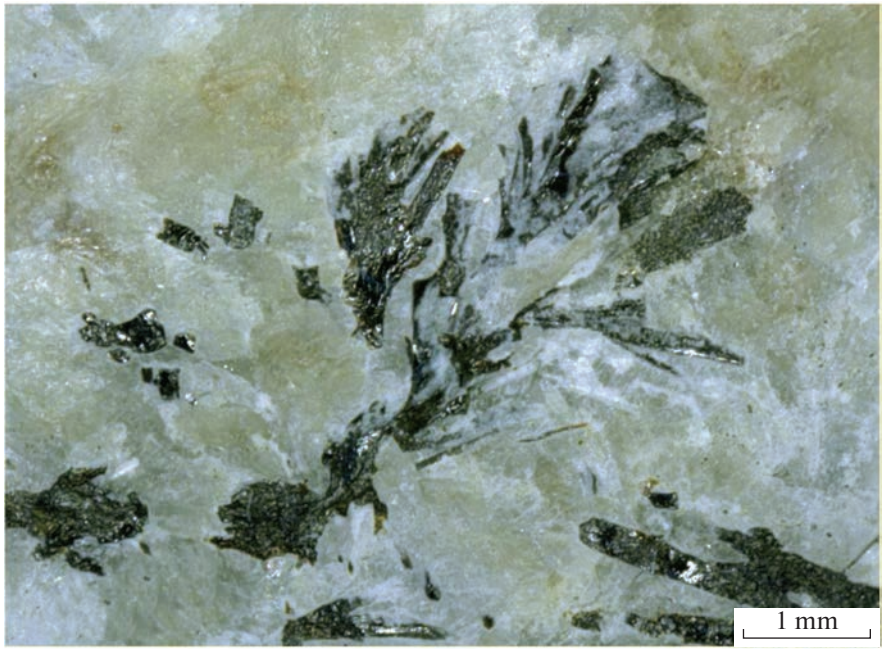

Fig. 1. Aggregates of nioboixiolite-(Mn^{2+}) in albite.

Рис. 1. Агрегаты ниобоиксиолита-(Mn^{2+}) в альбите.

The empirical formula of nioboixiolite-(Mn^{2+}) calculated on the basis of 8 oxygen atoms per formula unit (*apfu*) is $(Nb_{1.59}Mn^{2+}_{1.04}Ta_{0.59}Ti_{0.47}Sc_{0.13}Zr_{0.07}Y_{0.06}Sn_{0.03}U_{0.03}Fe^{3+}_{1.01})_{\Sigma 4.02}O_8$ ($Z = 1$). The total number of cations in this charge-balanced formula calculated on the anionic basis is very close to 4.00 *apfu* which confirms bivalent state of Mn. The number of electrons per cation site calculated from this formula is equal to 39.2 which is close to the value of 40.5 obtained as a result of the crystal structure refinement. The relative difference between these val-

Table 2. Reflectance values of nioboixiolite-(Mn^{2+})
Таблица 2. Коэффициенты отражения ниобоиксиолита-(Mn^{2+})

λ, nm	R_1	R_2	λ, nm	R_1	R_2
400	17.2	18.0	560	15.1	15.8
420	17.0	17.8	580	15.0	15.7
440	16.6	17.5	**589**	**15.0**	**15.66**
460	16.3	17.1	600	15.0	15.6
470	**16.1**	**16.9**	620	14.9	15.6
480	15.9	16.7	640	14.9	15.5
500	15.7	16.4	**650**	**14.9**	**15.5**
520	15.5	16.1	660	14.9	15.5
540	15.3	16.0	680	14.9	15.5
546	**15.3**	**15.9**	700	14.9	15.5

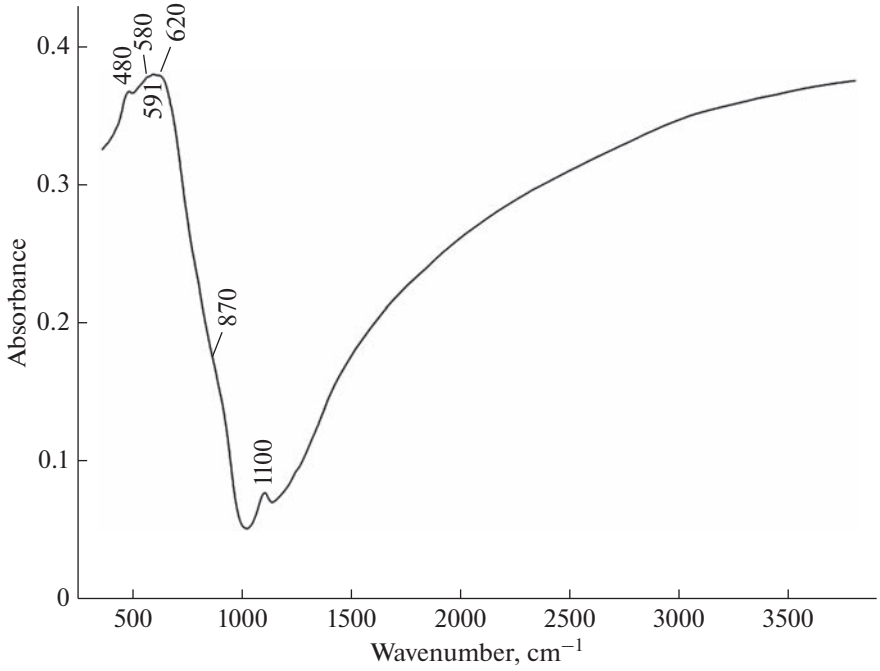

Fig. 2. Powder infrared absorption spectrum of nioboixiolite-(Mn^{2+}).

Рис. 2. Инфракрасный спектр поглощения порошка ниобоиксиолита-(Mn^{2+}).

ues is in the frame of the standard deviations in Table 3. The simplified formula is $(Nb,Mn^{2+},Ta,Ti)O_2$ and the formal, idealized end-member formula is $\left(Nb_{2/3}Mn^{2+}_{1/3}\right)O_2$.

3.3. X-ray diffraction data and crystal structure. Powder X-ray diffraction data of nioboixiolite-(Mn^{2+}) are given in Table 4. The orthorhombic unit-cell parameters refined from the powder data are: $a = 4.762(2)$ Å, $b = 5.739(1)$ Å, $c = 5.149(1)$ Å, $V = 140.7(1)$ Å^3.

Table 3. Chemical composition of nioboixiolite-(Mn^{2+})
Таблица 3. Химический состав ниобоиксиолита-(Mn^{2+})

Constituent	Average content, wt %	Range of contents, wt %	Standard deviation	Probe Standard
MnO	14.94	13.28–16.30	0.91	Mn
Sc_2O_3	1.80	1.31–2.06	0.26	Sc
Fe_2O_3	0.20	0.09–0.26	0.05	Pyroxene Hyp-746
Y_2O_3	1.34	0.93–2.59	0.59	Y
TiO_2	7.66	5.43–10.16	1.56	Ti
ZrO_2	1.74	0.51–2.66	0.73	Zr
SnO_2	1.01	0.43–1.99	0.40	Sn
ThO_2	0.26	0.00–0.98	0.37	ThO_2
UO_2	1.44	0.62–3.75	1.05	UO_2
Nb_2O_5	42.80	38.54–46.33	2.38	Nb
Ta_2O_5	26.77	24.71–28.48	1.15	Ta
Total	**99.96**			

Table 4. Powder X-ray diffraction data of nioboixiolite-(Mn^{2+})
Таблица 4. Порошковая рентгенограмма ниобоиксиолита-(Mn^{2+})

I_{obs}, %	d_{obs}, Å	I_{calc}*, %	d_{calc}**, Å	*h k l*
29	**3.662**	31	3.660	110
100	**2.984**	100	2.980	111
14	2.868	7	2.866	020
14	2.573	15	2.567	002
21	**2.505**	17	2.502	021
8	2.380	8	2.378	200
5	2.262	2	2.259	102
9	2.217	4	2.215	121
11	2.105	9	2.102	112
7	1.916	5	1.912	022
7	1.832	5	1.830	220
21	**1.775**	13	1.773	130
28	**1.748**	15	1.745	202
35	**1.726**	21	1.724	221
20	**1.553**	13	1.550	113
7	1.492	4	1.490	222
19	**1.473**	8	1.469	023
30	**1.463**	10, 12	1.464, 1.459	311, 132
4	1.435	1	1.433	040
7	1.382	5	1.380	041
3	1.316	2	1.313	312
2	1.288	2	1.284	004
5	1.252	3	1.250	223

* For the calculated pattern, only reflections with intensities ≥1 are given.
** For the unit-cell parameters calculated from single-crystal data; the strongest reflections are marked in boldtype.

The crystal structure of nioboixiolite-(Mn^{2+}) was refined using the SHELX software package (Sheldrick, 2015) to $R = 0.0474$ using 151 unique reflections with $I > 2\sigma(I)$ in the frame of space group *Pbcn*. The crystal data and the experimental details are presented in Table 1, atom coordinates, displacement parameters and site occupancies in Table 5. Selected interatomic distances are given in Table 6.

Nioboixiolite-(Mn^{2+}) is a representative of the α-PbO_2 structure type. The structure (Fig. 3) is based on the zig-zag chains of edge-sharing octahedra MO_6 (the major *M* cations are Nb, Mn, Ta, and Ti), running along the *c* axis. Adjacent chains are linked in *a* direction *via* common oxygen vertices. All cations are disordered and fill a single *M* site.

4. DISCUSSION

The Nb-dominant structural analogue of ixiolite was described in several publications (von Knorring and Sahama, 1969; Wise *et al.*, 1998; Badanina *et al.*, 2008; Alekseev *et al.*, 2010; Zubkova *et al.*, 2020), usually as ixiolite (or its varieties, scandian ixiolite, wolframo-ixiolite, *etc.*), despite the prevailing of Nb over Ta. So-called "ashanite" initially described as a Nb-dominant analogue of ixiolite (Zhan Rubo *et al.*, 1980) has been discredited by the IMA CNMMN be-

Table 5. Coordinates and equivalent displacement parameters (U_{eq}, in Å^2) of atoms in the structure of nioboixiolite-(Mn^{2+})
Таблица 5. Координаты позиций и параметры атомных смещений (U_{eq}, Å^2) в структуре ниобоиксиолита-(Mn^{2+})

Site	*x*	*y*	*z*	U_{eq}
M	0.0	0.32861(19)	0.25	0.0191(5)
O	0.7270(14)	0.1132(11)	0.4170(14)	0.021(2)

The refined number of electrons at the *M* site is $e_{ref} = 40.52$.

Table 6. Cation-oxygen distances (Å) in the structure of nioboixiolite-(Mn^{2+})
Таблица 6. Расстояния катион–кислород в структуре ниобоиксиолита-(Mn^{2+})

M–O 1.984(7) × 2
–O 2.052(8) × 2
–O 2.137(7) × 2
Mean 2.058

cause of unfair chemical data, corresponding to a mixture of several minerals, presumably ixiolite, samarskite-(Y), and uranmicrolite (Ganfu Shen, 1998; Jambor *et al.*, 1999).

An overwhelming majority of finds of ixiolite and its Nb-dominant analogue, forming a continuous isomorphous series, is related to Li-F granites and, especially, rare-element granitic pegmatites. All samples of ixiolite series minerals from these formations contain sig-

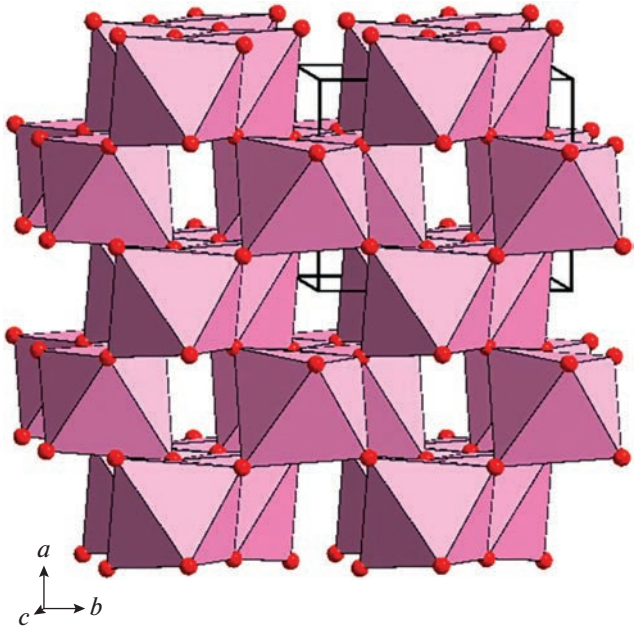

Fig. 3. The crystal structure of nioboixiolite-(Mn^{2+}). The unit cell is outlined.

Рис. 3. Кристаллическая структура ниобоиксиолита-(Mn^{2+}). Показана элементарная ячейка.

Table 7. Comparative data of nioboixiolite-(Mn^{2+}) and closely related minerals
Таблица 7. Сравнительные данные для ниобоиксиолита-(Mn^{2+}) и родственных ему минералов

Mineral	Nioboixiolite-(Mn^{2+})	Ixiolite-(Mn^{2+})	Columbite-(Mn)
Idealized formula	$(Nb_{2/3}Mn^{2+}{}_{1/3})O_2$	$(Ta_{2/3}Mn^{2+}{}_{1/3})O_2$	$Mn^{2+}Nb_2O_6$
Crystal system Space group	Orthorhombic *Pbcn*	Orthorhombic *Pbcn*	Orthorhombic *Pbcn*
a, Å *b*, Å *c*, Å *V*, Å^3 *Z*	4.7559 5.7318 5.1344 139.97 4	4.74–4.76 5.70–5.74 5.10–5.16 138.4–140.6 4	14.433 5.7637 5.0832 422.86 4
Strongest reflections of the powder X-ray diffraction pattern: *d*, Å (*I*, %)	3.662 (29) 2.984 (100) 2.505 (21) 1.775 (21) 1.748 (28) 1.726 (35) 1.463 (30)	3.65 (32) 2.98 (100) 2.57 (13) 2.51 (20) 1.746 (17) 1.722 (24) 1.459 (29)	3.678 (90) 2.985 (100) 2.880 (50) 2.505 (50) 1.905 (60) 1.840 (60) 1.776 (60)
Density, g cm^{-3}	5.803 (calc.)	6.94–7.23 (meas.) 7.392 (calc.)	5.20–6.65 (meas.) 5.30 (calc.)
References	This work	Nickel et al., 1963; Černý and Němec, 1995; Chukhrov and Bonshtedt-Kupletskaya, 1967	Wise and Černý, 1984; Wise et al., 1985; Mineralogy..., 2000

nificant amounts of Ta. Some of them contain U and/or Th admixtures and are partly or completely metamict.

The crystal structure of a natural niobium analogue of ixiolite was first published only recently, for an unusual Ta- and Sn-free and Ti- and Fe-rich sample from the Eifel paleovolcanic region, Germany (Zubkova et al., 2020), but a detailed investigation of this sample was not carried out because of scarcity of available material.

Synthetic Nb-dominant oxides isostructural with ixiolite are described in a number of works. In particular, the crystal structures of the compounds $Fe^{3+}NbO_4$–II (Harrison and Cheetham, 1989), $\left(Nb_xFe^{3+}_xZn_{1-x}\right)(O_{4x}F_{2-2x})$ (with x from 0.75 to 1.00: Pourroy et al., 1990), and Nb_2TiZnO_8 (Baumgarte and Blachnik, 1992) have been investigated. All of them belong to the α-PbO_2 structure type.

Comparative data for nioboixiolite-(Mn^{2+}) and closely related minerals are given in Table 7. Nioboixiolite-(Mn^{2+}) is chemically related to columbite-(Mn), $Mn^{2+}Nb_2O_6$, and can be considered as a cation-disordered analogue of this mineral.

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НИОБОИКСИОЛИТ-(Mn^{2+}) $\left(Nb_{2/3}Mn^{2+}_{1/3}\right)O_2$ – НОВЫЙ МИНЕРАЛ ГРУППЫ ИКСИОЛИТА ИЗ МАЛХАНСКОГО ПЕГМАТИТОВОГО ПОЛЯ, ЗАБАЙКАЛЬЕ

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Новый минерал группы иксиолита, ниобоиксиолит-(Mn^{2+}) с идеализированной формулой $\left(Nb_{2/3}Mn^{2+}_{1/3}\right)O_2$, ниобиевый аналог иксиолита-(Mn^{2+}), найден в гранитном пегматите жилы Соседка (Малханское пегматитовое поле, Забайкальский край) в ассоциации с альбитом, кварцем, микроклином, эльбаитом, бериллом, висмутином, эвксенитом-(Y), цирконом, рутилом, касситеритом и каннонитом. Новый минерал образует вросшие в альбит радиальные сростки призматических кристаллов с размерами до 0.8 × 1.5 × 5 мм. Цвет ниобоиксиолита-(Mn^{2+}) темно-коричневый до черного, блеск металловидный до алмазного, черта коричневая. Спайность не наблюдается. Твердость по шкале Мооса 4.5–5. Вычисленная плотность 5.803 г/см^3. Даны ИК-спектр и спектр отражения в видимой области. Химический состав ниобоиксиолита-(Mn^{2+}) (по данным электронно-зондовых анализов, мас. %): MnO 14.94, Sc_2O_3 1.80, Fe_2O_3 0.20, Y_2O_3 1.34, TiO_2 7.66, ZrO_2 1.74, SnO_2 1.01, ThO_2 0.26, UO_2 1.44, Nb_2O_5 42.80, Ta_2O_5 26.77, сумма 99.96. Эмпирическая формула: $(Nb_{1.59}Mn^{2+}_{1.04}Ta_{0.59}Ti_{0.47}Sc_{0.13}Zr_{0.07}Y_{0.06}Sn_{0.03}U_{0.03}Fe^{3+}_{0.01})_{\Sigma 4.02}O_8$ (Z = 1). Кристаллическая структура решена на монокристалле и уточнена до R = 0.0474. Ниобоиксиолит-(Mn^{2+}) изоструктурен с другими членами группы иксиолита. Новый минерал ромбический, пространственная группа *Pbcn*, параметры элементарной ячейки равны a = = 4.762(2) Å, b = 5.739(1) Å, c = 5.149(1) Å, V = 140.7(1) Å^3. Наиболее сильные линии порошковой рентгенограммы [*d,* Å (*I*, %) (*hkl*)]: 3.662 (29) (110), 2.984 (100) (111), 2.505 (21) (021), 1.775 (21) (130), 1.748 (28) (202), 1.726 (35) (221), 1.553 (20) (113), 1.473 (19) (023), 1.463 (30) (311, 132).

Ключевые слова: ниобоиксиолит-(Mn^{2+}), новый минерал, группа иксиолита, надгруппа колумбита, кристаллическая структура, Малханское пегматитовое поле