Columbite supergroup of minerals: nomenclature and classification

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Abstract

The columbite supergroup is established. It includes five mineral groups (ixiolite, wolframite, samarskite, columbite, and wodginite) and one ungrouped species (lithiotantite). The criteria for a mineral to belong to the columbite supergroup are: the general stoichiometry MO_2; the crystal structure based on the hexagonal close packing (*hcp*) of anions (or close to it); the six-fold coordination number of *M*-type cations (augmented to eight-fold in the case of slight distortion of *hcp*); and the presence of *zig-zag* chains of edge-sharing *M*-centered polyhedra. The ixiolite-type structure is considered as an *aristotype* with the space group *Pbcn*, the smallest unit cell volume, and the basic vectors $\mathbf{a_0}$, $\mathbf{b_0}$, $\mathbf{c_0}$. Based on the multiplying of the ixiolite-type unit cell the following derivatives are distinguished: ixiolite type (ixiolite-group minerals; $a = \mathbf{a_0}$, $b = \mathbf{b_0}$, $c = \mathbf{c_0}$; *Pbcn*; the members are ixiolite-(Mn^{2+}), ixiolite-(Fe^{2+}), scrutinyite, seifertite, and srilankite), wolframite type (wolframite-group minerals, ordered analogs of the ixiolite type with $a = \mathbf{a_0}$, $b = \mathbf{b_0}$, $c = \mathbf{c_0}$; *P*2/*c*; the members are ferberite, hübnerite, huanzalaite, sanmartinite, heftetjernite, nioboheftetjernite, rossovskyite, and andriesite), samarskite type (samarskite-group minerals; $a = 2\mathbf{a_0}$, $b = \mathbf{b_0}$, $c = \mathbf{c_0}$; *P*2/*c*; the members are samarskite-(Y), ekebergite, and shakhdaraite-(Y)), columbite type (columbite-group minerals; $a = 3\mathbf{a_0}$, $b = \mathbf{b_0}$, $c = \mathbf{c_0}$; *Pbcn*; the members are columbite-(Fe), columbite-(Mn), columbite-(Mg), tantalite-(Fe), tantalite-(Mn), tantalite-(Mg), fersmite, euxenite-(Y), tanteuxenite-(Y), and uranopolycrase), and wodginite type (wodginite-group minerals; $a = 2\mathbf{a_0}$, $b = 2\mathbf{b_0}$, $c = \mathbf{c_0}$; *C*2/*c*; the members are wodginite, ferrowodginite, titanowodginite, ferrotitanowodginite, tantalowodginite, lithiowodginite, and achalaite). Samarskite-(Yb), ishikawaite, and calciosamarskite are insufficiently studied minerals tentatively considered as possible members of the samarskite supergroup. Qitianlingite, yttrocolumbite-(Y), yttrotantalite-(Y), and yttrocrasite-(Y) are questionable minerals which need further studies. Polycrase-(Y) is discredited as a mineral identical with euxenite-(Y). Ixiolite has been renamed to ixiolite-(Mn^{2+}), with the end-member formula $(Ta_{2/3}Mn^{2+}_{1/3})O_2$. Ta- and Nb-dominant analogues of ixiolite with different schemes of charge balancing have the end-member formulae $(M1^{5+}_{0.5}M2^{3+}_{0.5})O_2$,

$M1^{5+}{}_{2/3}M2^{2+}{}_{1/3})O_2$, $M1^{5+}{}_{0.75}M2^{+}{}_{0.25})O_2$ or $M1^{5+}{}_{0.8}\square_{0.2})O_2$ and the root name "ixiolite" (for $M1$ = Ta) or "nioboixiolite" (for $M1$ = Nb).

Keywords: columbite supergroup, ixiolite group, wolframite group, samarskite group, columbite group, wodginite group, lithiotantite, nomenclature, classification.

Introduction

Among Ti^{4+}-, Sn^{4+}-, $^{VI}Ge^{4+}$-, ^{VI}Si-, $^{VI}Mn^{4+}$-, $^{VI}Pb^{4+}$-, $^{VI}Te^{4+}$-, Nb-, Ta-, Sb^{5+}-, Mo^{6+}- and W^{6+}-oxide minerals with the stoichiometry MO_2, there are numerous mineral species structurally related to columbite. Although they display substantial common features, these minerals differ from each other in many aspects including different kinds of cation ordering, symmetry, unit-cell dimensions, and coordination numbers of cations. Attempts to elaborate a general crystal-chemical classification of columbite-type minerals and other related mineral species with the stoichiometry MO_2 have been undertaken repeatedly (Graham and Thornber, 1974a; Sugitani *et al*., 1985; Hanson *et al*., 1999). This paper summarizes available data on the minerals with the stoichiometry MO_2 that are topologically related to columbite and constitute the columbite supergroup. The nomenclature and classification of the columbite supergroup has been approved by the IMA Commission on New Minerals, Nomenclature and Classification.

The root-name columbite is the oldest one among all names of mineral species that are discussed in this nomenclature report. Minerals belonging to the columbite group are important from the petrological, geochemical and practical points of view.

The name is after the chemical composition: the mineral columbite was originally described as an iron and columbium oxide. Columbium is an older and today obsolete name for the chemical element that later was re-named niobium. The mineral, however, retained its name. The root columbium is also maintained in "coltan", an acronym which refers to the niobium/tantalum oxides.

General Definitions

The following criteria are applied to define the minerals of the columbite supergroup:

I. The general stoichiometry MO_2 is required.

II. The crystal structure is based on the hexagonal close packing (*hcp*) of anions (or close to it).

III. Only octahedral voids of *hcp* are occupied. As a result, the coordinational number of *M*-type cations is 6 (sometimes augmented to 8 in the case of slight distortion of *hcp*).

IV. The presence of *zig-zag* chains of edge-shared octahedra (the idealized symmetry described by the rod group $\not{p}2/c11$; Fig. 1).

The application of these criteria obviously excludes compounds with rutile-related structures (*e.g*. tapiolite-group minerals) which are characterized by straight chains of edge-sharing octahedra with the idealized symmetry described by the rod group $\not{p}112/m$ (Fig. 1). Alumotantite (Ercit *et al*., 1992d) matches only the criteria I-III and is not considered as a member of the columbite supergroup. A short outline of minerals with the general MO_2 stoichiometry which do not belong to the columbite supergroup (and as such were not part of the IMA-approved report) has been deposited with the Principal Editor of Mineralogical Magazine and is available as Supplementary material (see below).

Using the approach applied for the perovskite supergroup (Mitchell *et al*., 2017), the ixiolite-type structure is considered as an *aristotype* with the space group *Pbcn* and the smallest unit cell volume and the basic vectors $\mathbf{a}_0$, $\mathbf{b}_0$, $\mathbf{c}_0$. Based on the multiplying of the initial ixiolite-type unit cell the following derivatives can be distinguished (Fig. 2a):

- **ixiolite type** with $a = \mathbf{a}_0, b = \mathbf{b}_0, c = \mathbf{c}_0$; *Pbcn*;
- **wolframite type** (an ordered analog of the ixiolite type) with $a = \mathbf{a}_0, b = \mathbf{b}_0, c = \mathbf{c}_0$; *P*2/*c*;
- **samarskite type** with $a = 2\mathbf{a}_0, b = \mathbf{b}_0, c = \mathbf{c}_0$; *P*2/*c*;
- **columbite type** with $a = 3\mathbf{a}_0, b = \mathbf{b}_0, c = \mathbf{c}_0$; *Pbcn*;
- **wodginite type** with $a = 2\mathbf{a}_0, b = 2\mathbf{b}_0, c = \mathbf{c}_0$; *C*2/*c*.

Different schemes of ordering of *M* cations control both the symmetry lowering and multiplying of the basic ixiolite-type unit cell. The Bärnighausen tree (Müller, 2004) shown in Fig. 2b illustrates the symmetry relations between different structures.

Minerals belonging to the columbite supergroup

Ixiolite group

Minerals belonging to the ixiolite group with the general formula $M1O_2$ (orthorhombic, *Pbcn*, $a = \mathbf{a_0}$, $b = \mathbf{b_0}$, $c = \mathbf{c_0}$, $Z = 4$**)** are characterized by a disordered distribution of the cations: in the crystal structure of ixiolite-group minerals (Fig. 3), all cations occupy a single *M*1 site. In these minerals, edge-sharing $M1O_6$ octahedra form chains along the **c** direction. In the **a** direction, the chains are connected with each other *via* common vertices of the octahedra.

Ixiolite was first described by Nordenskiöld (1857) as a tantalum oxide, with subordinate Fe and Mn and minor Sn. The sample originated from Skogsböle, Kimito Island, Finland. The chemical analysis of the sample from Skogsböle is incomplete and corresponds to the approximate formula $Ta_{0.6}(Fe,Mn)_{0.3}Sn_{0.1}O_2$. The Fe:Mn ratio was not determined. Based on goniometric measurements, the mineral was assumed to be orthorhombic with a:b:c = 1:0.5508:1.2460. D_{meas} = 7.0 – 7.1. *H*(Mohs) = 6 – 6½.

In another ixiolite sample from Skogsböle, the Mn:Fe ratio is 1.04:1 in atomic units (Rose, 1858). Mn-rich ixiolite (with 9.35 wt.% MnO) has been also discovered in pegmatites of the Kalbinskiy range, Russia (Chukhrov and Bonshtedt-Kupletskaya, 1967). The crystal structure of Mn-rich ixiolite with the charge-balanced empirical formula $(Ta_{0.43}Nb_{0.24})Mn^{2+}_{0.23}Mn^{3+}_{0.07}(Ti_{0.02}Sn_{0.01})O_2$ from the Tanco pegmatite, Bernic Lake, Manitoba, Canada was solved by Grice et al. (1976).

The chemical formula of ixiolite is currently given as $(Ta,Mn,Nb)O_2$ which corresponds to an ixiolite-group mineral with Mn as the main charge-balancing component, but samples with Fe > Mn are also known. In most analyses of ixiolite from Skogböle, Fe prevails over Mn, with Fe:Mn up to 13.8:1 (Rose, 1858). Nickel et al. (1963a) investigated the crystal structure of an ixiolite sample from Skogböle with the charge-balanced empirical formula $(Ta_{0.43}Nb_{0.12})(Fe^{2+}_{0.13}Mn^{2+}_{0.12})Fe^{3+}_{0.05}(Sn_{0.13}Ti_{0.01}Zr_{0.01})O_2$. The sample is deposited in the Royal Ontario Museum with the catalogue number M-6591. The synthetic compound with the formula $NbFe^{3+}O_4$ and ixiolite-type structure was described by Harrison and Cheetham (1989).

Scrutinyite, α-PbO_2 was discovered in two natural occurrences situated in Bingham, New Mexico, USA and Mapimi, Mexico (Taggart et al., 1988). The crystal structure of synthetic α-PbO_2 was solved by Zaslavskij and Tolkachev (1952).

Seifertite, SiO_2, is an orthorhombic high-pressure silica polymorph with the ixiolite-type structure. The mineral is a constituent of high-pressure assemblages typical of shock-affected Martian meteorites belonging to the shergottite group (Dera *et al*., 2002; El Goresy *et al*., 2008; Zhang *et al*., 2016).

Srilankite, TiO_2, was described as a new mineral from Rakwana, Sabaragamuva province, Sri Lanka (Willgallis *et al*., 1983). The chemical composition was originally given as $(Ti,Zr)O_2$, with Zr:Ti = 1:2. The ixiolite-type structure of srilankite has been confirmed by a SCXRD study of natural sample (Willgallis and Hartl, 1983) and its synthetic analogue (Troitzsch *et al.*, 2005). Likewise transition metals in other ixiolite-group minerals, Ti and Zr in srilankite occupy the same crystallographic *M*1 site. Zirconium, having an ionic radius larger than titanium, plays an essential role in stabilizing the ixiolite-type structure of srilankite at ambient pressure. Zirconium-free srilankite, pure TiO_2, was described as a quenched “TiO_2-II” polymorph from the Ries impact structure (El Goresy *et al*., 2001), the Xiuyan crater in China (Zhang *et al*., 2009) and in the high-pressure mineral assemblages of subduction zones (Chen *et al*., 2013).

The Nb-dominant analogue of ixiolite (with Nb > Ta) has been known for a long time (von Knorring and Sahama, 1969; Wise *et al*., 1998; Zubkova *et al*., 2020). This mineral was described as the new mineral species ashanite with the formula $(Nb,Ta,U,Fe,Mn)_4O_8$ (Z = 1) (Zhan *et al*., 1980). However, in 1998, ashanite was discredited by the IMA Commission on New Minerals and

Mineral Names. This decision was made based on unsatisfactory compositional data for this mineral, suggestive of a mixture of ixiolite, samarskite, and uranmicrolite (Shen, 1998).

Although there is only one cationic $M1$ site in the ixiolite-type structure, charge-balanced end-member formulae of ixiolite and its Nb-dominant analogue cannot be written with a single cationic component. Thus, the dominant-charge-compensating cations (either a lower-valency cation or vacancy) should be taken into account, as discussed by Hatert and Burke (2008).

Wolframite group

The wolframite-type structure ($M1M2O_4$, monoclinic, $P2/c$, $a = \mathbf{a_0}$, $b = \mathbf{b_0}$, $c = \mathbf{c_0}$, $\beta \sim 91°$, $Z = 2$**)** is a derivative of the ixiolite-type structure characterized by the ordering of the cations with lowering of the symmetry. It can be represented as a sequence of two kinds of structurally identical, but chemically different, octahedral layers of parallel *zig-zag* chains alternating along the *a*-axis of ixiolite quasi-framework (Fig. 4). The larger-radius cations occupy the octahedral $M1$ site, whereas the smaller-radius cations reside at the $M2$ octahedron. Consequently, the members of the wolframite group are double oxides with the general formula $M1^{2+}M2^{6+}O_4$ ($M1$ = Mg, Mn, Fe, Zn; $M2$ = W) or $M1^{3+}M2^{5+}O_4$ ($M1$ = Sc, Fe; $M2$ = Nb, Ta). The $Ti^{4+}Ti^{4+}O_4$ oxide, riesite, represents a slightly distorted variant of the wolframite structure. The layer-wise ordering of different-sized cations in wolframites results in monoclinic distortion of the ixiolite framework, whereas the unit-cell dimensions of parent ixiolite remain unchanged.

The wolframite group inherits its name from *wolframite*, which is now considered to be an obsolete mineral species. The first scientific description of this mineral with the name “Wolfram” (“wolf-cream”, from German Wolfram or Wolfrahm) was made by Henckel (1725).

Historically, wolframites represent intermediate members of the solid solution between pure $Fe^{2+}WO_4$ and pure $Mn^{2+}WO_4$. In particular, the term wolframite indicated the minerals with the compositions ranging between $(Fe_{0.8}Mn_{0.2})WO_4$ and $(Fe_{0.2}Mn_{0.8})WO_4$. The species having Fe > 0.8 and Mn > 0.8 atoms per formula unit (*apfu*) were called ferberite and hübnerite, respectively.

Subsequently, compositional fields of ferberite and hübnerite have been expanded according to the 50% rule and the term “wolframite” has been abandoned. For historical reasons, however, it seems convenient to keep wolframite as the name for the group of ordered structures with ixiolite-type unit cell, but with the space group *P*2/*c*.

Ferberite was first described by Liebe (1863). The type locality is the Niña mine, Sierra Almagrera, Andalusia, Spain. The crystal structure of ferberite has been refined by Cid-Dresdner and Escobar (1968).

Hübnerite was first described by Credner (1865). The type locality is the Ellsworth mine, Nevada, USA. The crystal structure of ferberite has been refined by Dachs *et al*. (1967).

Huanzalaite is the Mg-dominant analogue of ferberite and hübnerite. It was first described by Miyawaki *et al.* (2010). The type locality is the Huanzala mine, Ancash Department, Peru. The crystal structure of its synthetic analogue has been refined by Macavei and Schulz (1993).

Sanmartinite, ideally $ZnWO_4$, was first described by Angelelli and Gordon (1948). The type locality is the Department of San Martín, San Luis province, Argentina. The crystal structure of sanmartinite has been refined by Redfern *et al*. (1995).

Heftetjernite, $ScTaO_4$, was first described by Kolitsch *et al*. (2010), who also refined its crystal structure. The type locality is the Heftetjern pegmatite, Tørdal, Telemark, Norway.

Nioboheftetjernite, $ScNbO_4$, was first described by Lykova *et al*. (2021), who also refined its crystal structure. The type locality is the Befanamo pegmatite, Madagascar.

Rossovskyite was first described by Konovalenko *et al*. (2015), who also refined its crystal structure. The type locality is Bulgut, Altai Mountains, Mongolia. The chemical formula of the mineral is given as $(Fe^{3+},Ta)(Nb,Ti)O_4$. According to the dominant-valency rule and the site total charge approach (Bosi *et al*., 2019), the end-member formula is $Fe^{3+}NbO_4$.

Riesite was reported as a new TiO_2 polymorph from impact-affected rocks (suevites) at the Ries impact crater, Germany (Tschauner *et al*., 2020). Like formerly described Zr-free srilankite, riesite was formed by shock-induced transformation of rutile at pressures of 20–25 GPa. In the crystal structure of riesite, the *M*1 and *M*2 sites are insignificantly displaced from the general positions of the wolframite-type framework, becoming statistically half-occupied. By analogy with other wolframite-group minerals, the ideal formula of riesite can be written as $TiTiO_4$.

Samarskite group

The samarskite group includes three valid species, namely, samarskite-(Y), ekebergite, and shakhdaraite-(Y). These minerals are monoclinic (space group *P*2/*c*, 2$\mathbf{a}_0$: $\mathbf{b}_0$: $\mathbf{c}_0$, β ~ 93°; *Z* = 2), cation-ordered double niobates and tantalates with the general formula $AM1M2_2O_8$ (*A* = Y, Th; *M*1 = Fe^{2+}, Fe^{3+}, Sc^{3+}; *M*2 = Nb, Ta) and unit-cell parameters *a* = 9.8 – 9.9, *b* = 5.6 – 5.7, *c* ~ 5.2 Å, and β = 92 – 94 ° (*Z* = 2). Unlike other columbite-supergroup minerals, members of the samarskite group contain a relatively large cation at the *A* site with 6+2-fold coordination (Fig. 6) due to the slight distortion of the *hcp* (Lima-de-Faria, 2012). Such insertion of large cation transforms parallel zig-zag chains into a rigid layer of edge-sharing AO_8 polyhedra with the preservation of the cation distribution between the "octahedral" voids of *hcp* (Fig. 7). There are also three insufficiently studied metamict minerals, namely, samarskite-(Yb), ishikawaite, and calciosamarskite, that are tentatively assigned to the samarskite group based on their stoichiometry and the PXRD patterns of annealed samples.

The name samarskite was introduced into the mineralogical literature by Rose (1847) who described a sample from Ilmen Mountains, Chelyabinsk region, Russia. Then, the mineral name was changed to samarskite-(Y) according to general nomenclature rules for the *REE*-bearing minerals (Levinson, 1966). According to Hanson *et al*. (1999), the name samarskite-(Y) is attributed to the samarskite-group mineral in which the *A* site is dominated by *REE* cations, among which Y^{3+} prevails.

Samarskite-(*Y*) is the first member of the samarskite group whose crystal structure was published. A recent finding of non-metamict samarskite-(Y) allowed the refinement of its crystal structure, and the re-definition of the mineral as $YFe^{3+}Nb_2O_8$ (Britvin *et al*., 2019). These authors confirmed that this new chemical formula, with Fe^{3+} as a species-forming constituent, corresponds to the formula of holotype samarskite-(Y).

Ekebergite, ideally $ThFe^{2+}Nb_2O_8$, was approved as a new mineral species in 2018 (Kjellman *et al*., 2018). This mineral originates from the pumice quarry “In den Dellen” (Bimsgrube Zieglowski), Mendig, Laacher See (Laach Lake) complex, Eifel, Rhineland-Palatinate, Germany. Ekebergite is isostructural with samarskite and forms a solid-solution series with samarskite. The full description of the mineral has not as yet been published.

Shakhdaraite-(*Y*), $YScNb_2O_8$, was described as a new mineral from Tajikistan (Pautov *et al*., 2022). It is the Sc-dominant analogue of samarskite-(Y).

Samarskite-(*Yb*), $YbFe^{3+}Nb_2O_8$, was described as a new mineral by Simmons *et al*. (2006). It occurs as a metamict mineral at the Little Patsy pegmatite, South Platte district, Jefferson Co., Colorado, USA. The mineral recrystallized after heating at 1100°C for 12 h.

Ishikawaite was first described as an unnamed mineral from Ishikawa, Iwaki province, Japan, by Shimata and Kimura (1922a) and then named ishikawaite after the type locality (Shimata and Kimura, 1922b). Its chemical formula is currently given as $(U,Fe,Y)NbO_4$. According to Hanson *et al*. (1999), the name ishikawaite should be attributed to the samarskite-group mineral in which the *A* site is dominated by U^{4+}. Under this assumption, ishikawaite should be considered as the analogue of ekebergite with $U^{4+} > Th$ and the end-member formula $U^{4+}Fe^{2+}Nb_2O_8$.

Calciosamarskite was first described by Ellsworth (1928a, 1928b) as the Ca-dominant analogue of samarskite. Its chemical formula is currently given as $(Ca,Fe,Y)(Nb,Ta,Ti)O_4$. The mineral was supposed to be discredited (see Hanson *et al*., 1999), but actually it is still considered a valid, grandfathered species. According to Hanson *et al*. (1999), the name calciosamarskite should be attributed to the samarskite-group mineral in which the *A* site is dominated by Ca. However, the end-member formula $CaFe^{3+}Nb_2O_8$, which would be expected for a Ca-dominant samarskite-group mineral, is not charge-balanced even with trivalent iron. The formula $CaFe^{3+}Nb_2O_7(OH)$ is neutral, but the presence of OH groups in calciosamarskite is questionable. Probably, this problem could be solved based on data for the synthetic analogue.

Columbite group

The columbite group includes double oxides with the general formula $M1^{2+}M2^{5+}{}_2O_6$ (orthorhombic, *Pbcn,* $3\mathbf{a}_0 : \mathbf{b}_0 : \mathbf{c}_0$, $Z = 4$; $M1$ = Mg, Ca, Mn, Fe; $M2$ = Nb, Ta). In the crystal structure of these minerals (Fig. 8), $M1O_6$ octahedra share edges to form infinite *zig-zag* chains along the **c** axis. Similar chains are formed by the $M2O_6$ octahedra. Thus, alternating [100] "layers" are formed: a single "layer" consisting of chains of $M1O_6$ octahedra and double "layers" comprising chains of $M2O_6$ octahedra. The chains of the neighboring layers are linked *via* common vertices.

Columbite-(*Fe*), $Fe^{2+}Nb_2O_6$, is the current name of the mineral originally described as "columbite" and later named ferrocolumbite. Columbite was first described by Jameson (1805). The type locality is likely to be either Haddam or Middletown, both in Connecticut, USA (*cf.* Dana 1892). The mineral was renamed to columbite-(Fe) after Burke (2008). The crystal structure of natural columbite-(Fe) from S. José de Safira, Minas Gerais, Brazil has been refined by Tarantino and Zema (2005).

Columbite-(*Mn*), $Mn^{2+}Nb_2O_6$, was first described by Dana (1892) under the name manganocolumbite. This mineral was initially considered to be a Mn-dominant variety of columbite. The mineral was renamed to columbite-(Mn) after Burke (2008). The crystal structure of natural columbite-(Mn) from Kragero, Norway has been refined by Tarantino and Zema (2005).

Columbite-(*Mg*), $MgNb_2O_6$, the Mg-dominant member of the columbite solid-solution series, was first found in the Muzeinaya vein, Gorno-Badakhshan, Tajikistan (Mathias *et al*., 1963). The mineral was originally named magnocolumbite and then renamed to columbite-(Mg) after Burke (2008). The crystal structure of synthetic $MgNb_2O_6$ has been refined by Pagola *et al*. (1997).

Tantalite-(*Fe*), $Fe^{2+}Ta_2O_6$, is the current name of the mineral originally described as "tantalite" and then named ferrotantalite. Tantalite was first described by Thomson (1836). The type locality is Upper Bear Gulch, Tinton pegmatite district, Lawrence Co., South Dakota, USA. The mineral was renamed to tantalite-(Fe) after Burke (2008). An overwhelming majority of analyzed tantalite-(Fe) samples contain significant amounts of Mn and/or Nb. Samples with the compositions close to the $Fe^{2+}Ta_2O_6$ end-member have the tapiolite structure (Ercit *et al*., 1995).

Tantalite-(*Mn*), $Mn^{2+}Ta_2O_6$, was first described as "manganotantalite", a Mn-dominant variety of tantalite by Nordenskiöld (1877). The type locality is the Utö Mines, Stockholm Co., Sweden. The mineral was renamed to tantalite-(Mn) after Burke (2008). The crystal structure of natural tantalite-(Mn) from the Tanco pegmatite, Manitoba, Canada has been refined by Grice *et al*. (1976).

Tantalite-(*Mg*), $MgTa_2O_6$, was described as a new mineral "magnesiotantalite" from Lipovka, Central Urals, Russia by Pekov *et al*. (2003). The mineral was renamed to tantalite-(Mg) after Burke (2008).

Similarly to the samarskite type structures (Fig. 7), the insertion of cations with large ionic radii into the columbite-type structure causes the parallel *zig-zag* chains to transform into a rigid layer. Such layers of edge-shared AO_8-polyhedra (A = Ca, Y) have been found in the euxenite-derivative of the columbite type structure, where they alternates with double "layers" containing *zig-zag* chains of $M2O_6$ octahedra (Fig. 9). Despite the distortion of the initial *hcp*, the distribution of the cations over the "octahedral" void in the euxenite-derivative are exactly equal to those in the columbite-type structure (Lima-de-Faria, 2012).

Fersmite, $CaNb_2O_6$, was discovered in the pegmatites of the Vishnevye Mountains, Central Urals (Bohnstedt-Kupletskaya and Burova, 1946). The crystal structure of fersmite was solved by Aleksandrov (1960). The presumed synthetic analogue of fersmite is orthorhombic, space group *Pcan*, a 5.75, b 14.03, c 5.20 Å; $Z = 4$ (Cummings and Simonsen, 1970). Unlike other tantalite-group minerals, fersmite contains a rather large Ca cation having 8-fold coordination. Fersmite is dimorphous with the aeschynite-group mineral vigezzite.

Based on the stoichiometry, PXRD patterns of annealed samples and crystal structures of presumed synthetic analogues, four minerals whose natural samples are usually metamict [namely, euxenite-(Y), polycrase-(Y), tanteuxenite-(Y) and uranopolycrase] can be tentatively assigned to the columbite group (Palache *et al*., 1944; Weitzel and Schröcke, 1980; Aurisicchio *et al*., 1993).

Euxenite-(*Y*) is orthorhombic, with the end-member formula $YNbTiO_6$ and unit-cell parameters a ~14.6, b ~5.55, c ~5.2 Å. For example, the empirical formula of euxenite-(Y) from Lyndoch Township, Ontario, Canada (Ellsworth, 1927) calculated on 2(Nb+Ta+Ti+Fe^{3+}+Al) *apfu* is $[(Ca_{0.31}Fe^{2+}_{0.04}Mn_{0.02}Pb_{0.01})(Y_{0.58}Ce_{0.10})(Th_{0.07}U_{0.01})][(Fe^{3+}_{0.06}Al_{0.01})Ti_{0.74}(Nb_{1.13}Ta_{0.06})]O_{6.34}$. Numerous chemical data of euxenite-(Y) are given in the reference book Minerals (Chukhrov and Bonshtedt-Kupletskaya, 1967). All of them correspond to the end-member formula $YNbTiO_6$. The unit-cell parameters of a metamict euxenite-(Y) sample with the empirical formula $(\mathit{REE}_{0.92}Ca_{0.08}U_{0.11}Th_{0.06}Mn_{0.01})(Nb_{0.84}Ta_{0.09}Ti_{0.84}Fe_{0.12})O_6$ from a rare-metal pegmatite, which was annealed at 900°C, are a ~14.68, b ~5.56, c ~5.18 Å (Sokolova, 1959). The unit-cell parameters of synthetic $YNbTiO_6$ (Weitzel and Schröcke, 1980) are a 14.64, b 5.55, and c 5.20 Å.

Polycrase-(Y) which was considered as an analogue of euxenite-(Y) with Ti > Nb (in atomic units), is rarer. The empirical formula of metamict polycrase-(Y) from Birkenes, Norway is $(Y_{0.47}Ln_{0.20}Ca_{0.19}U_{0.18}Th_{0.06})$ $(Ti_{1.19}Nb_{0.71}Ta_{0.07})$ O_6 (Tomašić *et al*., 2004).

Non-metamict polycrase-(Y) with the unit-cell parameters a 14.82, b 5.66, c 5.22 Å was described by Guastoni *et al*. (2019). It occurs in the Fiume pegmatite dike, Vigezzo Valley, Central Alps, Italy. Its simplified empirical formula (analysis 9/1 in the cited paper) is $(Ca,Mn,Fe^{2+})_{0.085}\mathit{REE}_{0.78}(U,Th)_{0.19}Ti_{1.14}Si_{0.01}(Nb,Ta)_{0.78}W_{0.01}$.

Another sample described by Guastoni *et al*. (2019) originates from the Bosco dike situated in the same region. It is an intermediate member of the euxenite-(Y)–polycrase-(Y) solid-solution series and has the simplified formula $(Ca,Mn,Fe^{2+})_{0.165}\mathit{REE}_{0.84}(U,Th)_{0.10}Ti_{0.96}Si_{0.01}(Nb,Ta)_{0.96}W_{0.01}$. This sample is also non-metamict and has the unit-cell parameters a 14.736, b 5.605, c 5.184 Å. All available analyses of polycrase-(Y) correspond to the end-member formula $Y(NbTi)O_6$.

Thus, euxenite-(Y) and polycrase-(Y) (including those of annealed samples) are minerals with identical unit-cell parameters and the common end-member formula $Y(NbTi)O_6$. Consequently, these minerals should be considered as the same mineral species. The name euxenite-(Y), as the older of the two, has priority.

Tanteuxenite-(*Y*), $YTaTiO_6$, is a rare mineral first described from Western Australia (Simpson, 1928) and reported from a few other localities. The mineral is usually metamict.

Uranopolycrase, ideally UTi_2O_6, was described as a new mineral from Elba Island, Italy. Because the mineral is metamict, its crystal structure has been refined on a sample annealed at 900°C for 10 h (Aurisicchio *et al*., 1993).

Wodginite group

The wodginite group includes monoclinic minerals (space group $C2/c$; $2\mathbf{a}_0 : 2\mathbf{b}_0 : \mathbf{c}_0$, $\beta \sim 91°$, $Z = 4$) with the general formula $M1M2M3_2O_8$. The dominant cations at the M sites are: $M1 = Mn^{2+}, Fe^{2+}$, Li; $M2$ = Ti, Sn^{4+}, Ta; $M3$ = Ta. The structure of these minerals (Ercit *et al*., 1992a) is based on alternating (100) "layers" consisting of chains of edge-sharing MO_6 octahedra running along the **c** axis (Fig. 10). The "layers" of the first type contain chains of $M3O_6$ octahedra, whereas the "layers" of the second type contain chains of alternating $M1O_6$- and $M2O_6$ octahedra (Fig. 11). The chains of the neighboring layers are linked *via* common vertices. The structures of wodginite-group minerals are characterized by a different degree of the ordering of cations among the M sites; the heating of samples at 1000°C for 16 hours induces full order of cations in wodginite-group minerals (Ercit *et al*., 1992a,b,c).

Wodginite, ideally $MnSnTa_2O_8$, was described as a new mineral from two localities, Wodgina, Western Australia and Bernic Lake, Manitoba, Canada (Nickel *et al*., 1963b). Based on PXRD data, its crystal structure was recognized as a superstructure of ixiolite. The crystal-structure refinements have been carried out by Ercit *et al*. (1992a), who have shown that different samples have different degrees of Ta disorder. Partially ordered samples are structurally intermediate between wodginite and ixiolite. The crystal structure of wodginite from Wodgina was investigated by Graham and Thornber (1974b). Later, the crystal structure of wodginite from Bernic Lake was solved by Ferguson *et al*. (1976).

Ferrowodginite, $FeSnTa_2O_8$, was characterized as a new mineral species by Ercit *et al*. (1992c). In the type specimen, ferrowodginite occurs as 0.01- to 0.2-mm inclusions in cassiterite from a granitic pegmatite near Sukula, southwestern Finland.

Titanowodginite, $MnTiTa_2O_8$, holotype material occurs as euhedral crystals up to 1 cm across at the Tanco pegmatite, Bernic Lake, Manitoba, Canada. Its crystal structure was solved by Ercit *et al.* (1992c).

Ferrotitanowodginite, $FeTiTa_2O_8$, has been described from the San Elías pegmatite, Sierra de la Estanzuela, San Luis Province, Argentina (Galliski *et al*., 1999).

Tantalowodginite, $(Mn_{0.5}\square_{0.5})TaTa_2O_8$, was found in the Emmons granite pegmatite dike in Oxford County, Maine, USA (Hanson *et al*., 2018).

Lithiowodginite, $LiTa_3O_8$ or $LiTaTa_2O_8$, was discovered at the Ognevka and Yubileinoye tantalum deposits, Kalba Mountains, eastern Kazakhstan (Voloshin *et al*., 1990).

Achalaite, $Fe^{2+}TiNb_2O_8$, is the first Niobium-dominant member of the wodginite group and was described from the La Calandria granite pegmatite, Cañada del Puerto, Córdoba province, Argentina (Galliski *et al*., 2016).

Ungrouped columbite supergroup mineral

Lithiotantite, $LiTa_3O_8$, with space group $P2_1/c$, *a* 7.44 *b* 5.04 *c* 15.25 Å, $\beta = 107.2°$, $Z = 4$, is chemically and topologically identical to lithiowodginite (Fig. 12) (Voloshin *et al*., 1990; Ercit *et al*., 1992a,c).

Insufficiently studied minerals

The minerals listed below are not currently included in the columbite supergroup, pending reliable data on their chemical composition and crystal structure.

Qitianlingite is a mineral related to the members of the columbite and tantalite solid-solution series. It was described as a new mineral species with the ideal formula $Fe^{2+}_2Nb_2W^{6+}O_{10}$ (Yang *et al*., 1985). Qitianlingite was named after the type locality (Qitianling granite, Hunan Province, China). The crystal structure of qitianlingite has been refined by Peng *et al*. (1988), who described it as a superstructure of ixiolite with ordered cation distribution and a unit cell with the *a* axis approximately 5 times larger than the *a* axis of ixiolite (Fig. 12). However, calculated powder diffraction data confirming the superstructure of qitianlingite are not given in these papers. Indexing of all assumed superstructure reflections in the measured powder data is not in accordance with the pattern calculated from the proposed structure; all observed reflections can be indexed using an ixiolite-type cell. The holotype material of this mineral needs additional investigation.

Yttrocolumbite-(*Y*), $(Y,U,Fe^{2+})(Nb,Ta)(O,OH)_4$, is a questionable mineral described by Lepierre (1937). This mineral has been considered to be the Nb-dominant (with Nb > Ta) analogue of yttrotantalite-(Y). Natural yttrocolumbite-(Y) is metamict. The idealized formula of yttrocolumbite-(Y) coincides with those of fergusonite-(Y) and fergusonite-β-(Y).

Yttrotantalite-(*Y*) was described as a new mineral from Sweden (Ekeberg, 1802). Its chemical formula is currently given as $(Y,U,Fe^{2+})(Ta,Nb)(O,OH)_4$. Actually, its ideal chemical formula should be reduced to $YTaO_4$. Natural yttrotantalite-(Y) is metamict. It is considered a polymorph of formanite-(Y). Crystal structure refinements of yttrotantalite-(Y) have been carried out on presumed synthetic analogues; Keller (1962) described it with a samarskite-like unit cell, whereas Wolten (1967) described it with a wolframite-like unit cell.

Yttrocrasite-(Y) is an ill-defined mineral described as an yttrium-thorium-uranium titanate from the Burnet County, Texas, USA (Hidden and Warren, 1906). Its chemical formula is currently given as $(Y,Th,Ca,U)(Ti,Fe)_2(O,OH)_6$.

A mineral with the empirical formula $[\mathit{REE}_{0.52}(\mathrm{U,Th})_{0.25}(\mathrm{Fe}^{2+},\mathrm{Mn,Ca})_{0.20}]_{\Sigma 0.97}$ $[(\mathrm{Nb,Ta})_{1.26}\mathrm{Fe}^{3+}{}_{0.43}(\mathrm{Ti,Zr,Sn,Hf})_{0.28}\mathrm{W}_{0.03}]\mathrm{O}_6$ and with Y as the predominant *REE* was described by Nakajima and Kurosawa (2006) as "euxenite". If this sample is isostructural with euxenite, its end-member formula should be $\mathrm{Y(Nb_{1.5}Fe^{3+}{}_{0.5})O_6}$. Unfortunately, no X-ray diffraction data have been provided for this mineral.

Ginzburg et al. (1969) described a so-called "*wolframixiolite*" from an unknown locality. The empirical formula of this sample is $\mathrm{(Nb_{0.54}W_{0.46}Fe_{0.40}Mn_{0.30}Ta_{0.10}Zr_{0.06}U_{0.05}Ca_{0.03}Mg_{0.01}Ti_{0.01})O_4{\cdot}0.84H_2O}$. The powder diffraction data were indexed with a monoclinic cell *P*2/*c*, *a* 4.750, *b* 5.72, *c* 5.06 Å, β = 90º. A monoclinic cell was required because not all lines could be indexed with the ixiolite cell. Wang *et al*. (1988) described a homogeneous material with the composition $\mathrm{(Nb_{0.70}Fe_{0.50}W_{0.38}Mn_{0.23}Ta_{0.12}Ti_{0.03}Sn_{0.01})O_{4.00}}$, monoclinic, space group *Pc*, with *a* = 4.674, *b* = 3.673, *c* = 5.050 Å, and β = 90°. Borneman-Starynkevich *et al*. (1974), during a reinvestigation of the type material by electron microprobe analysis, found a Nb-Ta-Mn mineral without W as the main phase. The authors discuss whether wolframoixiolite is really a homogenous mineral or a mixture of ferberite with columbite. Eventually Nickel and Mandarino (1987) listed wolframoixiolite as a discredited mineral. Taking into account the relationships Nb > W, Fe + Mn > W, and Fe > Mn and under the assumption of a disordered cation distribution, the end-member formula of "*wolframixiolite*" could be $\mathrm{(Nb_{2/3}Fe^{2+}{}_{1/3})O_2}$. However, this mineral also needs additional investigation.

Summary of the approved report

a) Establishment of the supergroup

The columbite supergroup is established. It is divided into the ixiolite group, the wolframite group, the samarskite group, the columbite group, and the wodginite group.

b) Redefined species

Currently, IMA-accepted formulae of some mineral species belonging to the columbite supergroup do not correspond to their end-members. Introduction of end-member formulae for these minerals implies their redefinition. All these changes are summarized in Table 2.

c) Discredited species

The currently IMA-accepted formula for polycrase-(Y) is $Y(Ti,Nb)_2(O,OH)_6$. Its end member formula is $Y(NbTi)O_6$, which is identical to the revised formula of euxenite-(Y) (cf. Table 2). As euxenite (Scheerer, 1840) is older than polycrase (Scheerer, 1844), polycrase-(Y) should be discredited.

d) New species within the ixiolite group

As noted above, Nb-dominant analogues of ixiolite with different schemes of charge balancing are known from numerous localities. In order to distinguish minerals with different kinds of dominant charge-compensating cations (DCCC), the end-member formula will depend on the dominant cation within the dominant valence state of the charge-compensating cation. Accordingly, formulae will have the form:

for DCCC = 3+: $(Ta_{0.5}M^{3+}_{0.5})O_2$ and $(Nb_{0.5}M^{3+}_{0.5})O_2$

for DCCC = 2+: $(Ta_{2/3}M^{2+}_{1/3})O_2$ and $(Nb_{2/3}M^{2+}_{1/3})O_2$

for DCCC = 1+: $(Ta_{0.75}M^{+}_{0.25})O_2$ and $(Nb_{0.75}M^{+}_{0.25})O_2$

for DCCC = 0: $(Ta_{0.8}\square_{0.2})O_2$, and $(Nb_{0.8}\square_{0.2})O_2$

The DCCC will be appended to the root name "ixiolite" (for Ta-dominant end-members) or "nioboixiolite" (for Nb-dominant end-members). Accordingly:

- The current ixiolite will become ixiolite-(Mn^{2+}) with the formula $(Ta_{2/3}Mn^{2+}_{1/3})O_2$.
- Because Fe^{2+}-dominant "ixiolite" is also known to occur at the same locality (Rose, 1858; Nickel *et al.*, 1963), ixiolite-(Fe^{2+}) is now considered a distinct mineral species, with the formula $(Ta_{2/3}Fe^{2+}_{1/3})O_2$. The type locality for ixiolite-(Fe^{2+}) is Skogböle, Kimito, Finland. A similar procedure was recently adopted for the two grandfathered minerals "tetrahedrite" and "tennanite": both were redefined into two distinct species, after the IMA approved report on the tetrahedrite group (Biagioni *et al.,* 2020).

The unsuffixed names ixiolite and nioboixiolite will not refer to any specific mineral species and will get the status of series names.

The status of the ixiolite-related mineral qitianlingite remains unclear until more reliable data on the crystal structure of the holotype sample is solved.

e) Change of status

The crystal structures of three metamict minerals tentatively assigned to the samarskite group [namely, samarskite-(Yb), approved with the current formula $YbNbO_4$, ishikawaite, grandfathered with the current formula $(U,Fe,Y)NbO_4$, and calciosamarskite, grandfathered with the current formula $(Ca,Fe,Y)(Nb,Ta,Ti)O_4$] are unknown. Provided that these minerals are isostructural with samarskite-(Y), their end-member formulae could be written as $YbFe^{3+}Nb_2O_8$, $U^{4+}Fe^{2+}Nb_2O_8$, and $CaFe^{3+}Nb_2O_7(OH)$, respectively. However, before making effective the changes in their end-member formulae, all these minerals need further study and currently should be considered as questionable species; for instance, according to the type description of samarskite-(Yb) (Simmons *et al*., 2006), the mineral is iron-depleted, with only 0.11 Fe *apfu*, and all iron tentatively given as Fe^{2+}.

The status of yttrotantalite-(Y) is changed from Rn (renamed) to Q (questionable).

Appendix I

Topological features of columbite-supergroup minerals and crystal chemical isotypism between columbite-type structure and euxenite-type derivative

Ixiolite-, columbite-, wolframite-, and wodginite-group minerals as well as lithiotantite are characterized by the same topology of their atomic nets. Topological analysis of the octahedral frameworks in the columbite-supergroup members was performed based on a natural tiling (*i.e.* partition of the crystal space into the smallest cage-like units: Blatov *et al*., 2009) analysis of the 3*D* nets using the ToposPro software (Blatov *et al*., 2014). The atomic nets were simplified and the corresponding underlying nets, which characterize the connectivity of the primary structural units, were obtained. Topological analysis of the frameworks was performed based on a natural tiles analysis, where the tiles are the smallest clusters of the *3D* nets, and are characterized by the following set of tiles (Blatov *et al*., 2010): $[4.6^2]_2[6.8^2]_2[6^2.8^2]$ (Fig. A1). The further simplification of the 3*D* net using the *standard representation*, where only the centres (*M* cations) of the primary building units (**PBUs**) are retained in the underlying net, while the 3-connected ligands are pulled into edges, acting as bridges between the **PBUs** (Shevchenko and Blatov, 2021), gives the $[3^2.4^2]_2[3^4.4^2]$ set of tiles for the cationic 3*D* net (Fig. A1).

The analysis of the crystal-chemical similarity is a useful tool to analyze the crystal-chemical relation between different compounds with the same symmetry and unit-cell parameters for their systematics (Aksenov et al., 2021a, 2022a). In accordance with the nomenclature of inorganic structure types, two structures are defined as *configurationally isotypic* if: (i) they are *isopointal*[1] and (ii) for all corresponding Wyckoff positions, both the crystallographic point configurations and their geometrical interrelationships are similar (Lima-de-Faria *et al*., 1990). Comparison of the crystal structures of columbite-(Fe) (Balassone et al., 2015) with the columbite-type structure and fersmite (Gurbanova *et al*., 2001) with the euxenite-type derivative structure was done using the program *COMPSTRU* (de la Flor *et al*., 2016). In the crystal structures of both minerals, all the atoms fill the same Wyckoff positions. The calculated measure of similarity (Δ) (Bergerhoff *et al*., 1999) is 0.134 (Table A1). Thus, despite the difference in coordination environments and coordinational numbers of the *M*-sites, both minerals are configurationally isotypic. Similar crystal-chemical relations between structures characterized by different coordinational environments of the cation have been described *i.e.* for the natural and synthetic compounds with the general formula $A_2M_3(TO_4)_4$ (Aksenov *et al*., 2022).

Table A1. Table A1. Evaluation of the structure similarities between the columbite-type structure and euxenite-type derivative.

Minerals	Columbite-(Fe)	Fersmite

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[1] "*Two structures may be shown to be isopointal if they can be described in such a way that corresponding occupied Wyckoff positions have the same Wyckoff letters*" (Lima-de-Faria *et al*., 1990).

	(Balassone et al., 2015)	(Gurbanova *et al*., 2001)
S	0.0199	
d_{max} (Å)	0.4495	
d_{av} (Å)	0.2771	
Δ	0.134	
Transformation matrix (**P**, p)	**a**,**b**,**c**; ½, ½, 0	

Footnote:

The degree of lattice distortion (S) is the spontaneous strain (sum of the squared eigenvalues of the strain tensor divided by 3): $S = \frac{1}{3}\sqrt{\sum_{i=1}^{3} \eta_i^2}$, where η_i are the eigenvalues of the finite Lagrangian strain tensor (Cappilas *et al*., 2007). The d_{max} value is the maximal displacement between the atomic positions of the paired atoms, and d_{av} is the arithmetic mean of the distance (Orobengoa et al., 2009). The measure of similarity is $\Delta = \left[2^{1/2}\Delta(c) + 1\right]\Delta(d) - 1$, where $\Delta(c)$ is the sum of the weighted mean differences of the atomic coordinates of the structure 1 and 2; $\Delta(d)$ is the relation between the axial ratios of the structures 1 and 2.

Appendix II

Ixiolite-euxenite $(Eux)_n(Ixi)_m$-polysomatic series

The crystal structures with euxenite- and samarskite-type structure minerals are characterized by the presence of cations with the ionic radii > 0.9 Å (Y^{3+}, Th^{4+}, *etc*.), which leads to considerable distortion of the initial *hcp* and with the formation of the layer of edge-shared eight-vertex polyhedra (Voloshin, 1993; Capitani *et al*., 2016; Britvin *et al*., 2019). The increasing of the coordination number from 6 to 8 is in good agreement with values of valence sums for two additional bonds. This results in a significant transformation of the parental ixiolite-type topology.

In this case, in accordance with the published data on natural fersmite (as well as other members of euxenite group) and members of the samarskite group, these minerals should be considered as modular structures [by analogy with högbomite-group minerals composed by spinel

(*S*) and nolanite (*N*) modules; Armbruster, 2002], whose crystal structures are based on slightly distorted *hcp* and consist of two types of modules:

Euxenite (*Eux*) module: The "euxenite" (*Eux*) module has the general formula $[^{[8]}AO_2]$ and is represented by a central layer of edge-sharing AO_8-polyhedra (screwed cubes).

Ixiolite (*Ixi*) module: The single-layered "ixiolite" (*Ixi*) module with the general formula $[^{[6]}BO_2]$ is represented by *zig-zag* chains of edge-sharing BO_6-octahedra.

The occurrence of either of the above modules, or both, gives rise to the ixiolite-euxenite $(Eux)_n(Ixi)_m$-polysomatic series with the general formula $[^{[8]}AO_2]_n[^{[6]}BO_2]_m$ or $[^{[8]}A_n{}^{[6]}B_mO_{2(n+m)}]$. The polysomes are (Fig A2):

- **ixiolite type**, with $n = 0$, $m = 1$;
- **euxenite type**, with $n = 1$, $m = 2$;
- **samarskite type**, with $n = 1$, $m = 3$.

In general, the structure containing only *Eux*-modules ($n = 1$, $m = 0$) is characterized by a highly distorted fluorite-type topology (Sulyanova and Sobolev, 2022). However, direct link of two *Eux*-modules seems unlikely because of the considerable distortion of the AO_8 polyhedra (torsion angles in the polyhedra between the oxygen atoms of the adjacent *hcp* layers vary from 17° to 62°), accompanied by corresponding distortions of the oxygen layers. As a result, the distances and angles between the oxygen atoms of the same *hcp* layer become unsuitable for the formation of the square face of the AO_8-polyhedron of the adjacent *Eux*-module (Fig. A3).

The influence of the local heteropolyhedral substitutions on the topological features of the parental crystal structures has been previously shown (Aksenov et al., 2021b; 2022b). In the case of ixiolite-euxenite polysomatic series, the euxenite- and samarskite-type structures are characterized by the following tile sequences of the cationic 3*D* nets: $[3^4]_2[3^2.4^2]_4[3^4.4^2]_2[3^8]$ and $[3^4]_2[3^2.4^2]_6[3^4.4^2]_3[3^8]$, respectively. The tiles $[3^2.4^2]$ and $[3^4.4^2]$ are common for the all members of the polysomatic series.

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Figure captions

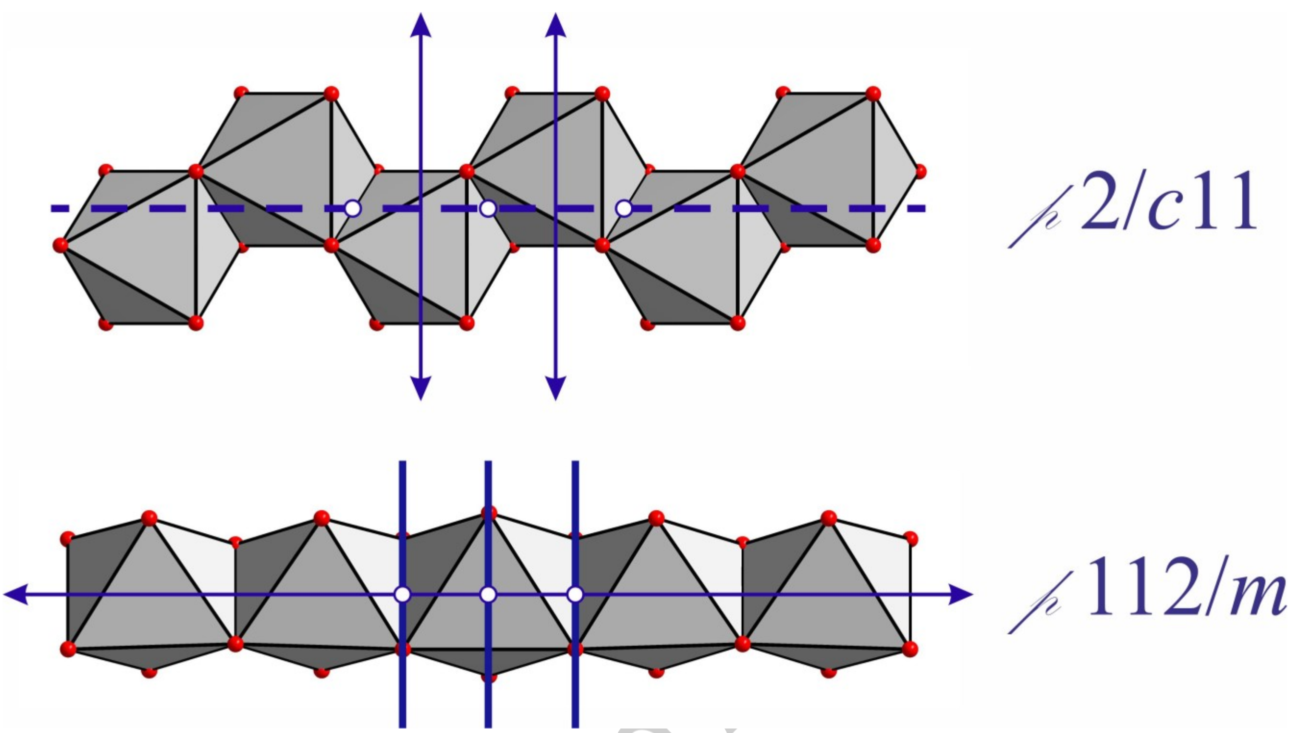
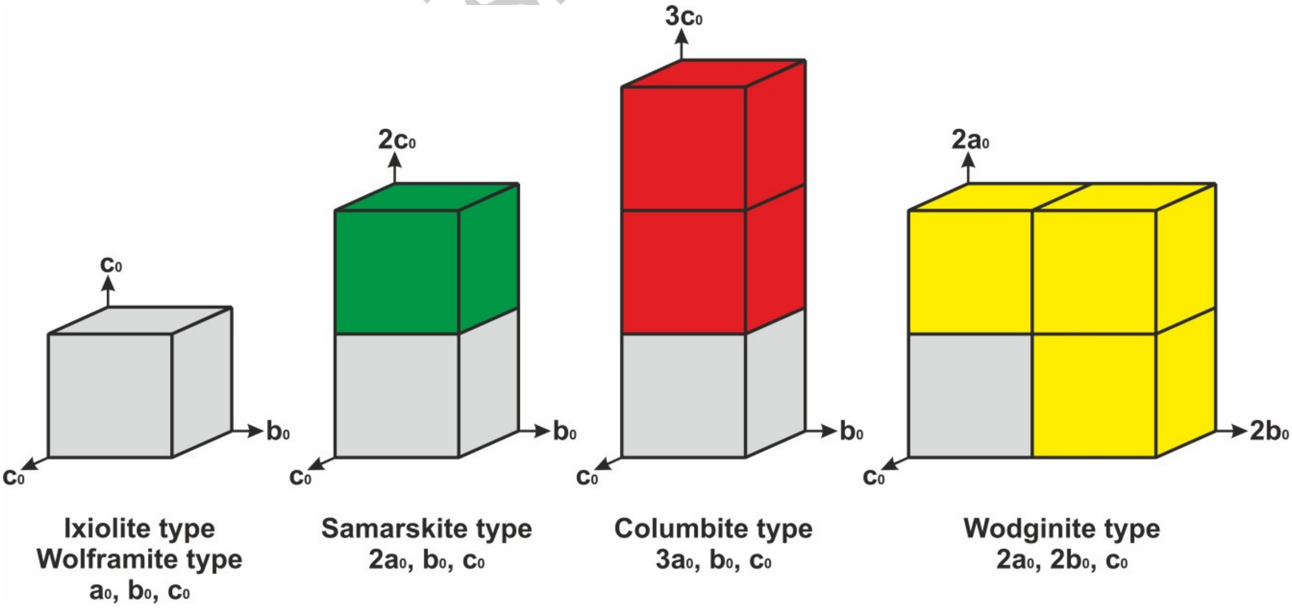


Fig. 1. The *zig-zag* and straight chains of edge-shared MO_6 octahedra and their rod groups.



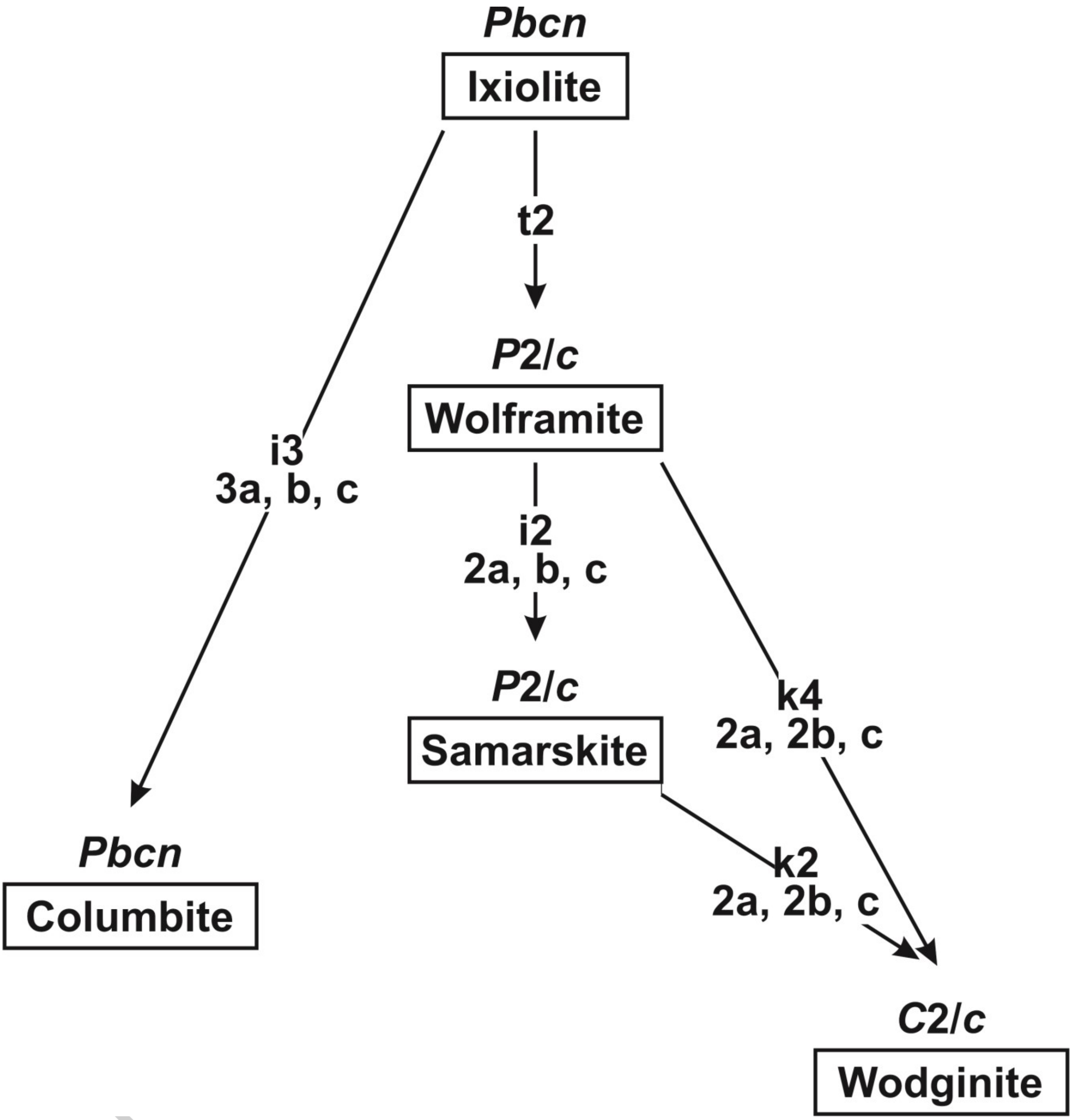


Fig. 2. General comparison of the unit cells (a), and symmetry reduction from the initial *aristotype* with the ixiolite-type unit cell and the space group *Pbcn* induced by the different kinds of ordering of cations (b).

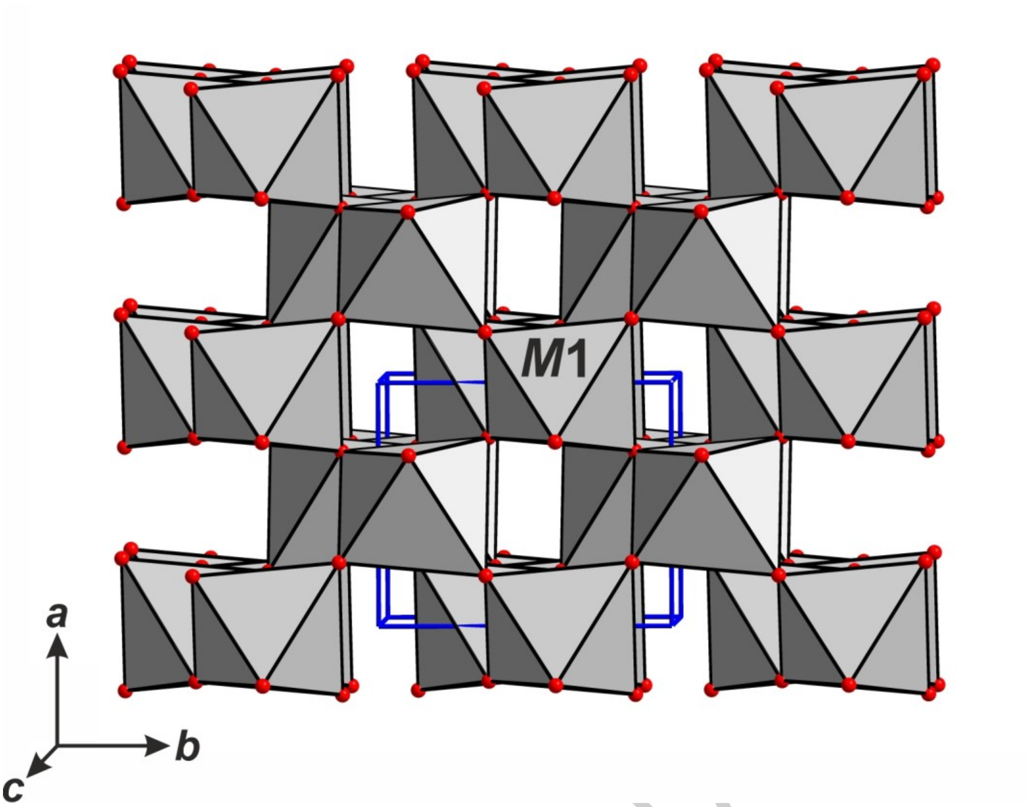


Fig. 3. The crystal structure of ixiolite-group minerals. The unit cell is outlined.

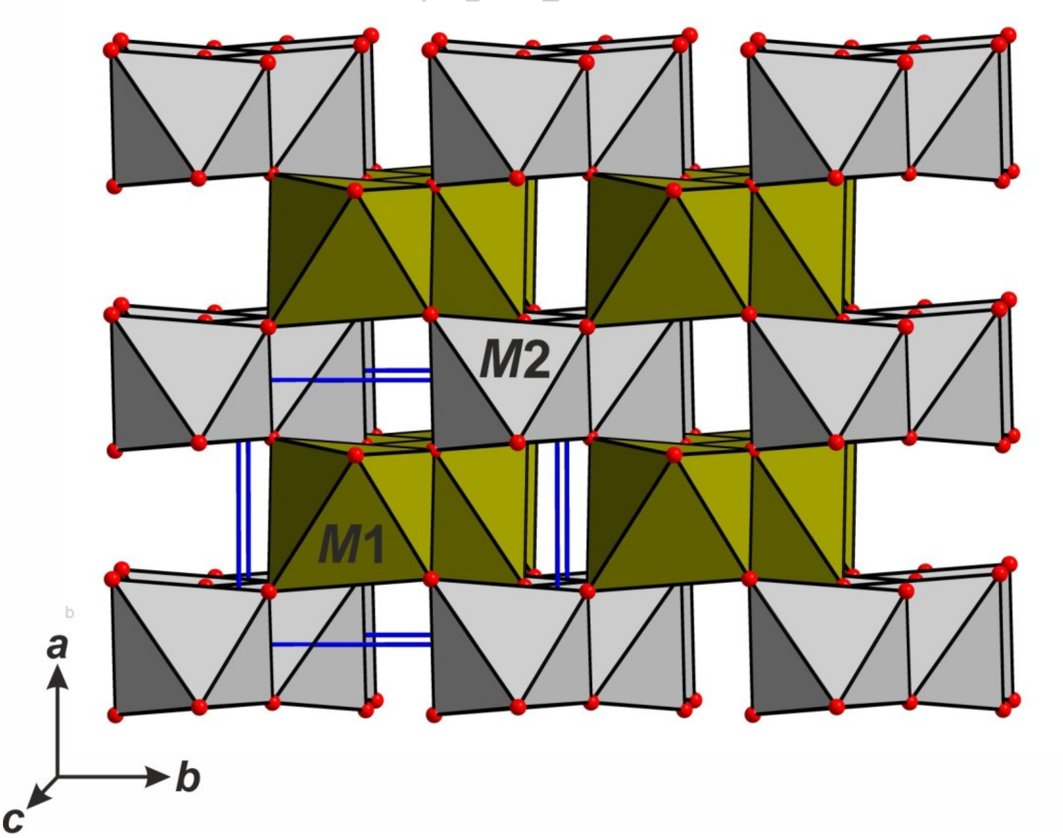
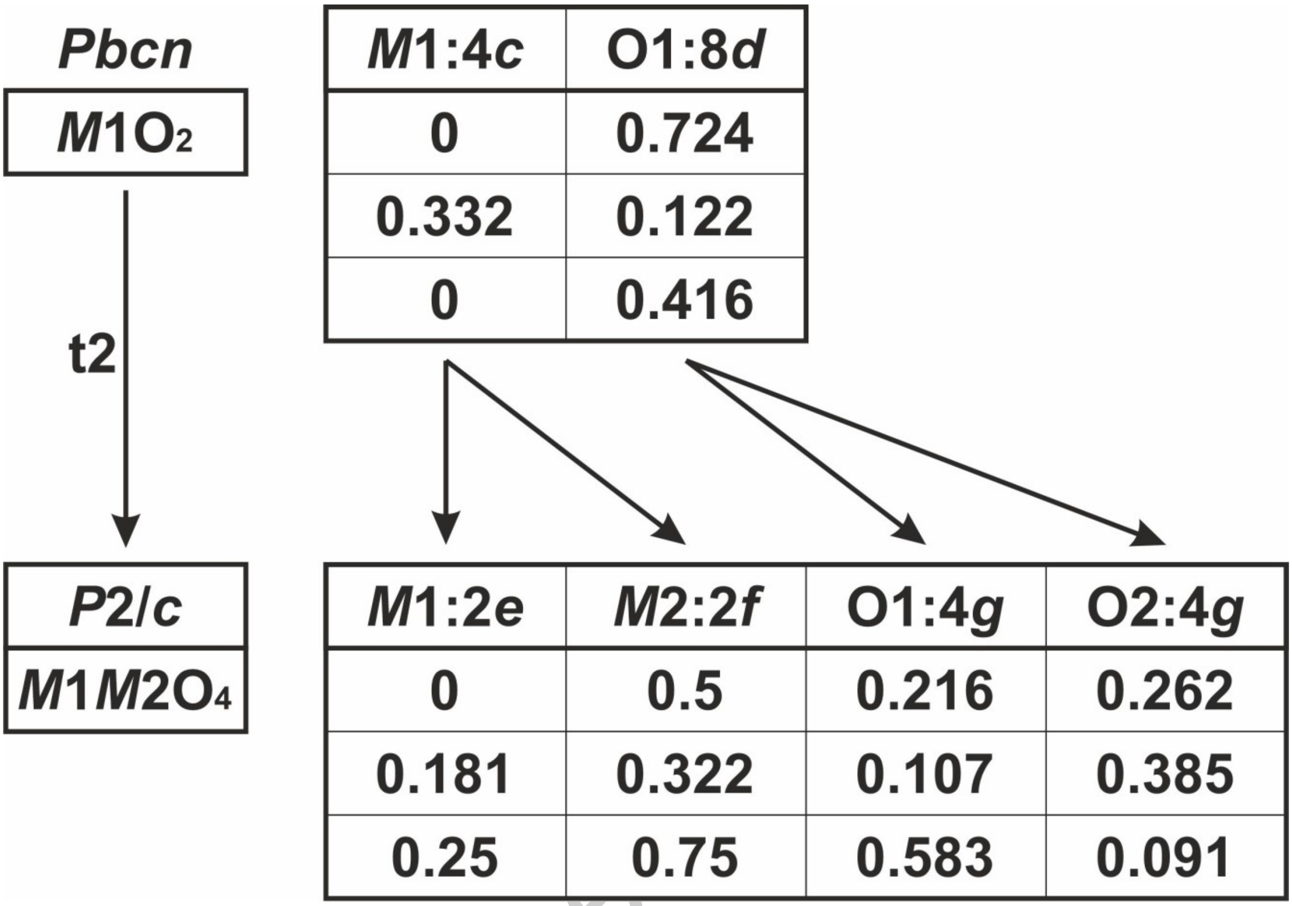


Fig. 4. General view of the wolframite-type structure.



*M*1:4*c*	O1:8*d*
0	0.724
0.332	0.122
0	0.416

*M*1:2*e*	*M*2:2*f*	O1:4*g*	O2:4*g*
0	0.5	0.216	0.262
0.181	0.322	0.107	0.385
0.25	0.75	0.583	0.091

Fig. 5. The scheme of splitting of atomic sites (the upper row) and their coordinates of the in the ixolite- and wolframite-type structures in accordance with the relations between the mineral groups (see Fig. 2b). One cationic *M*1 site and one oxygen O1 site in the ixiolite-type structure split into two symmetrically non-equivalent *M*1 and *M*2 as well as O1 and O2 sites in the wolframite-type structure due to the cation ordering and reducing of the symmetry from the space group *Pbcn* to *P*2/*c*.

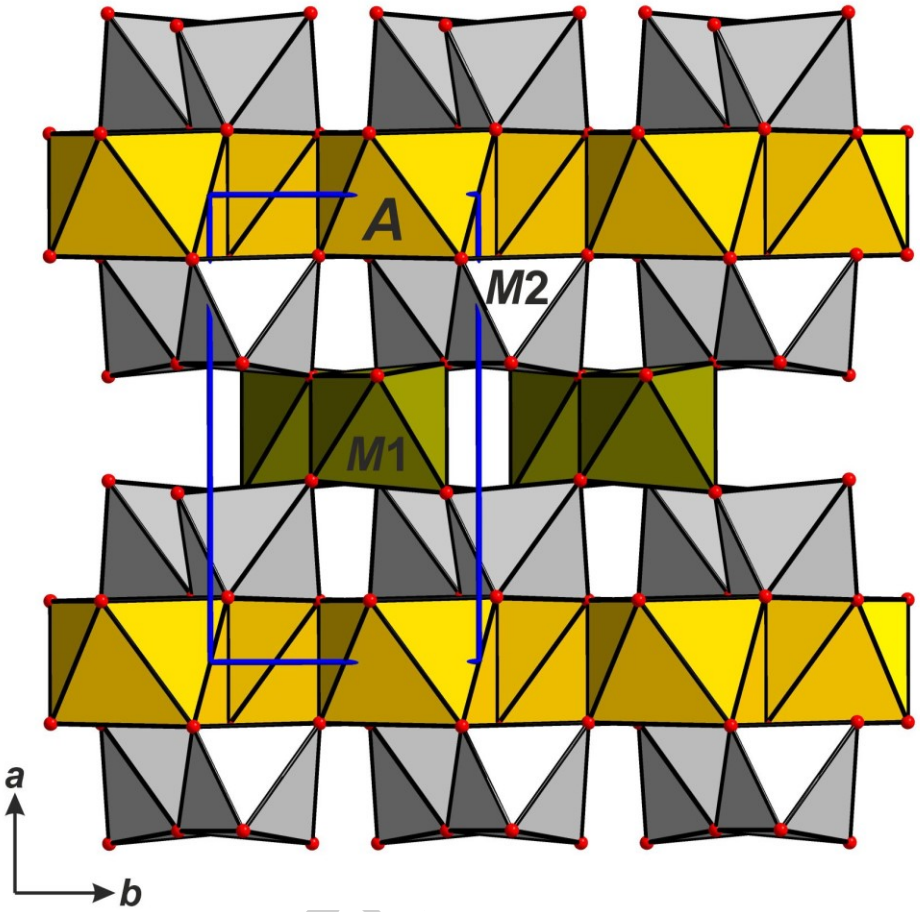


Fig. 6. General view of the samarskite-type structures.

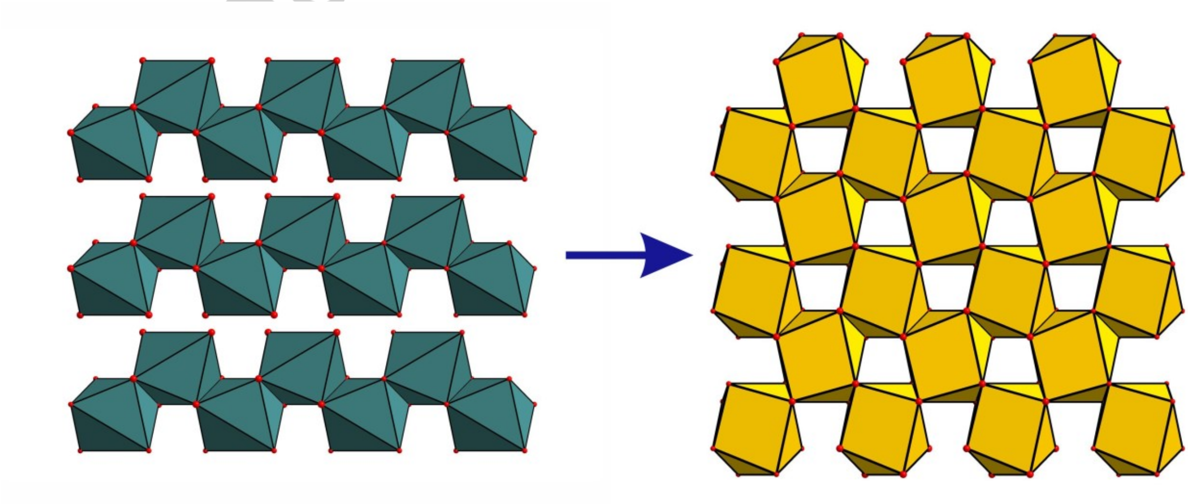


Fig. 7. Transformation of parallel *zig-zag* chains of edge-sharing octahedra into a solid layer of edge-shared eight-vertex polyhedra with the increasing of the ionic radii of the cation in the samarskite-type structures.

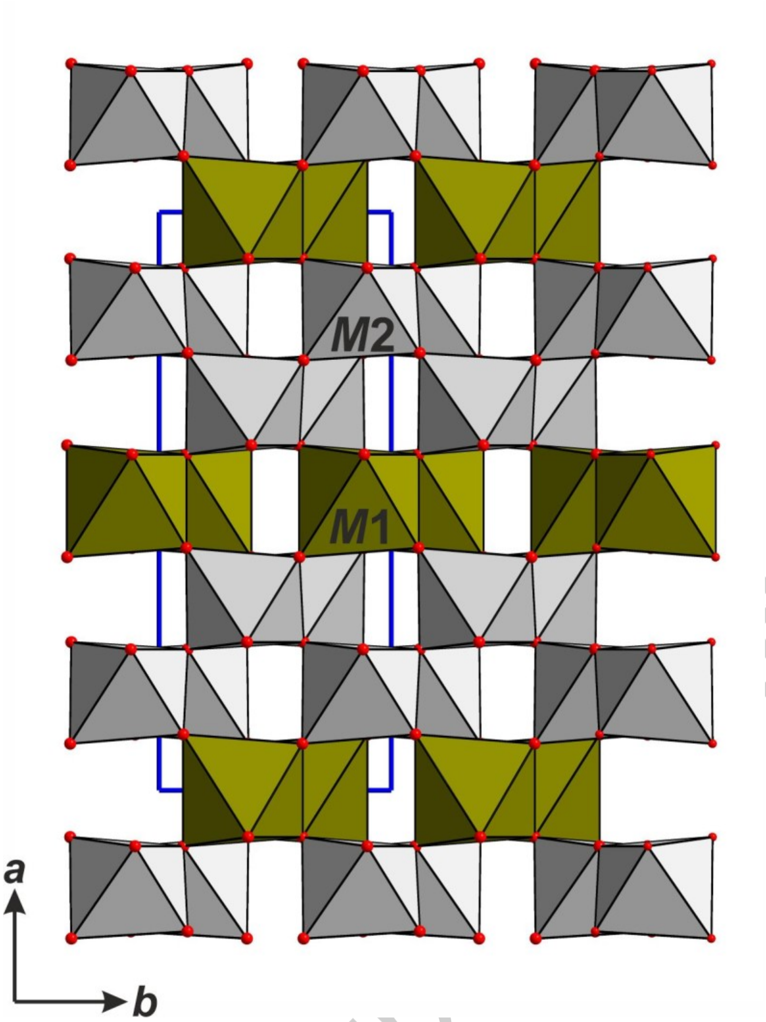


Fig. 8. The general view of the columbite-type structure. The unit cell is outlined.

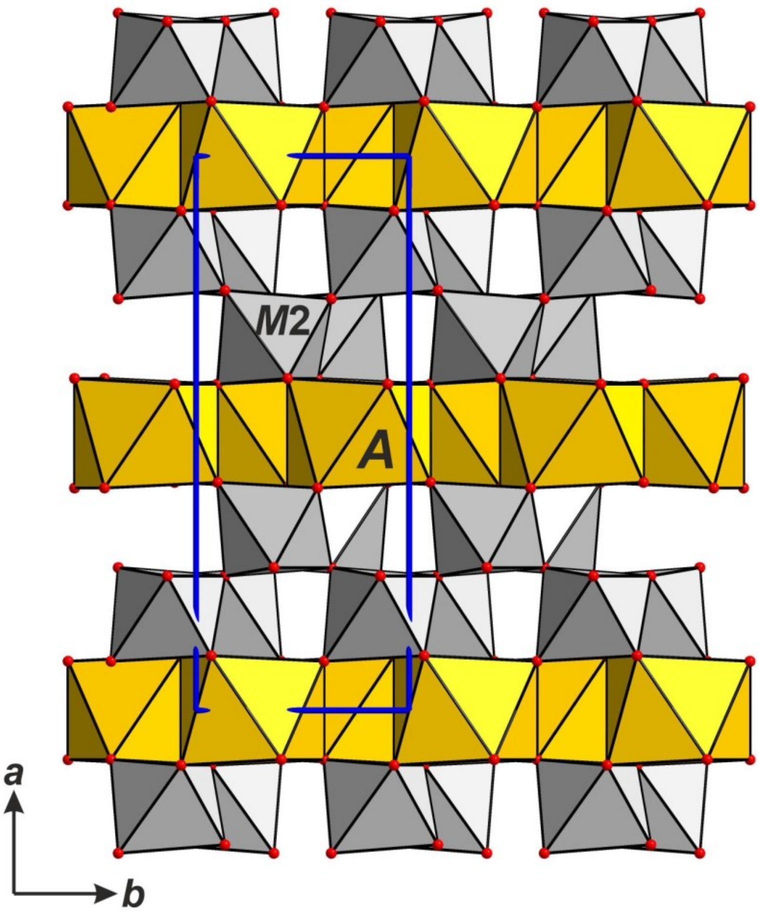


Fig. 9. General view of the euxenite-derivative of columbite-type structure containing layers of edge-shared eight-vertex polyhedra.

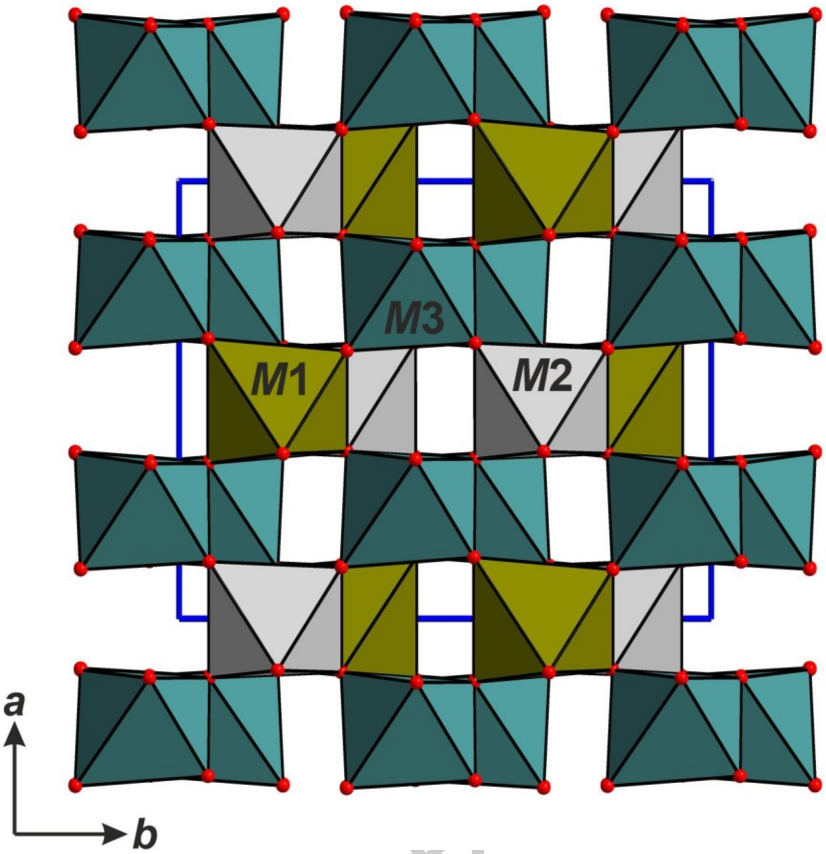


Fig. 10. General view of the wodginite-type structure.

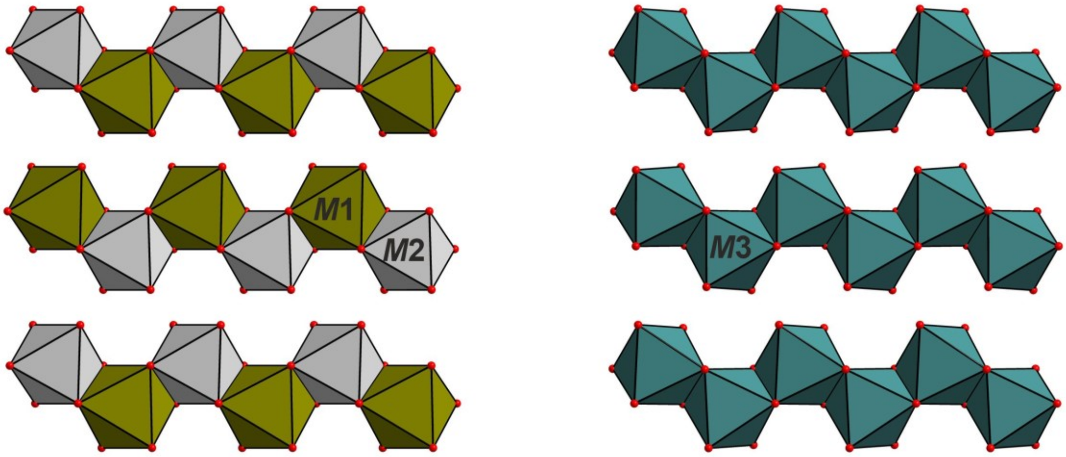


Fig. 11. Two types of layers containing zig-zag chains in the wodginite-type structure.

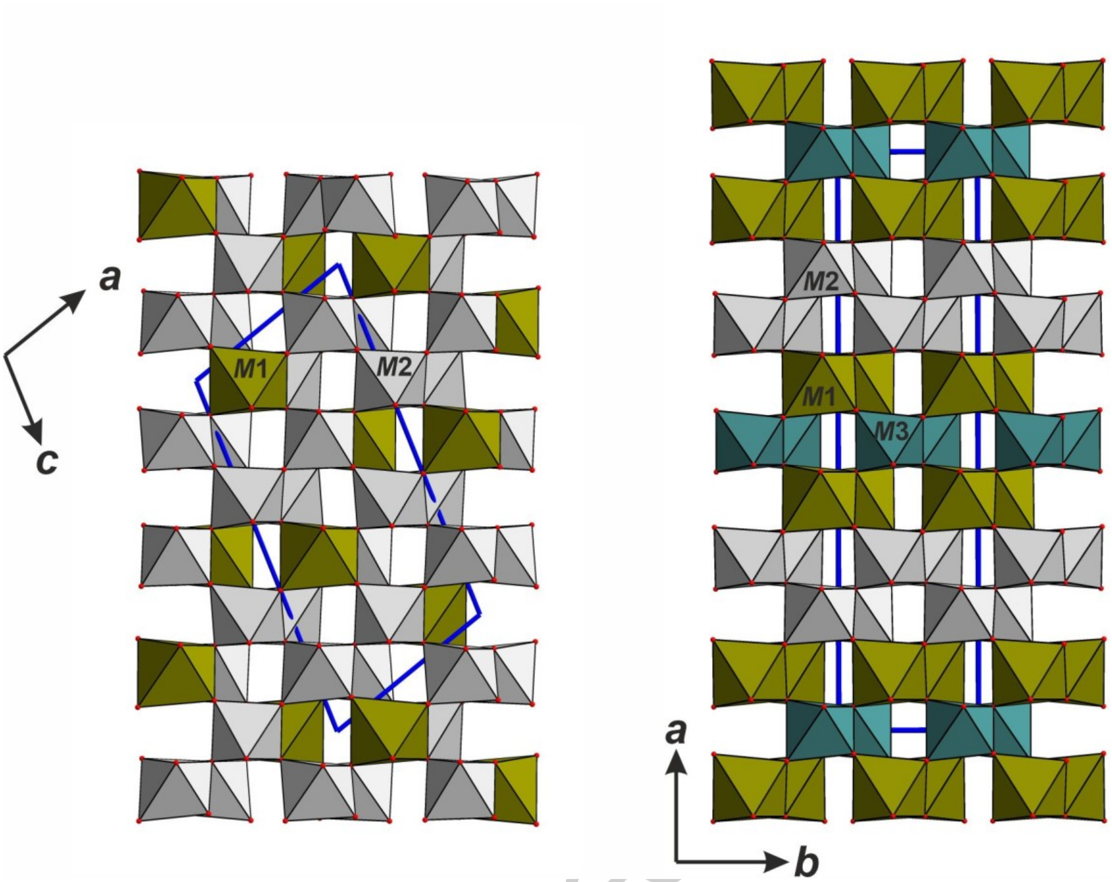


Fig. 12. The crystal structure of lithiotantite (left) and the proposed structure of qitianlingite (right).

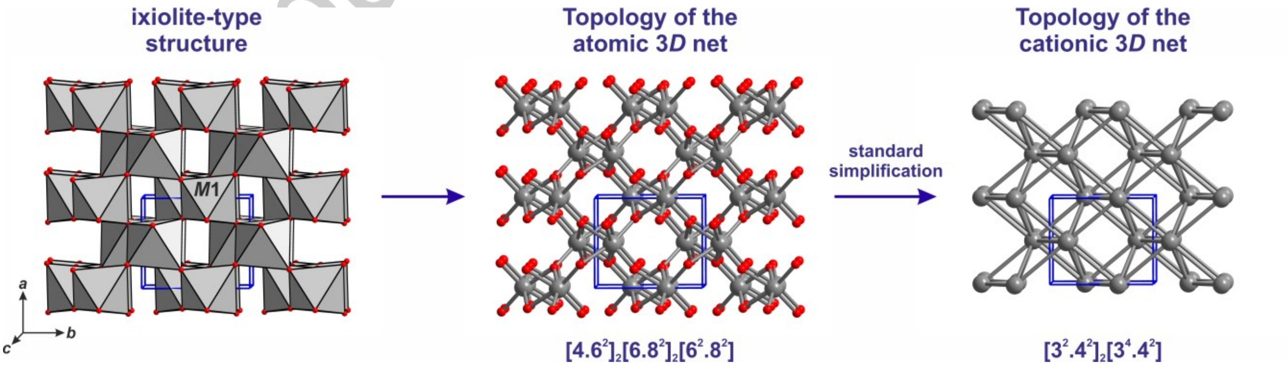
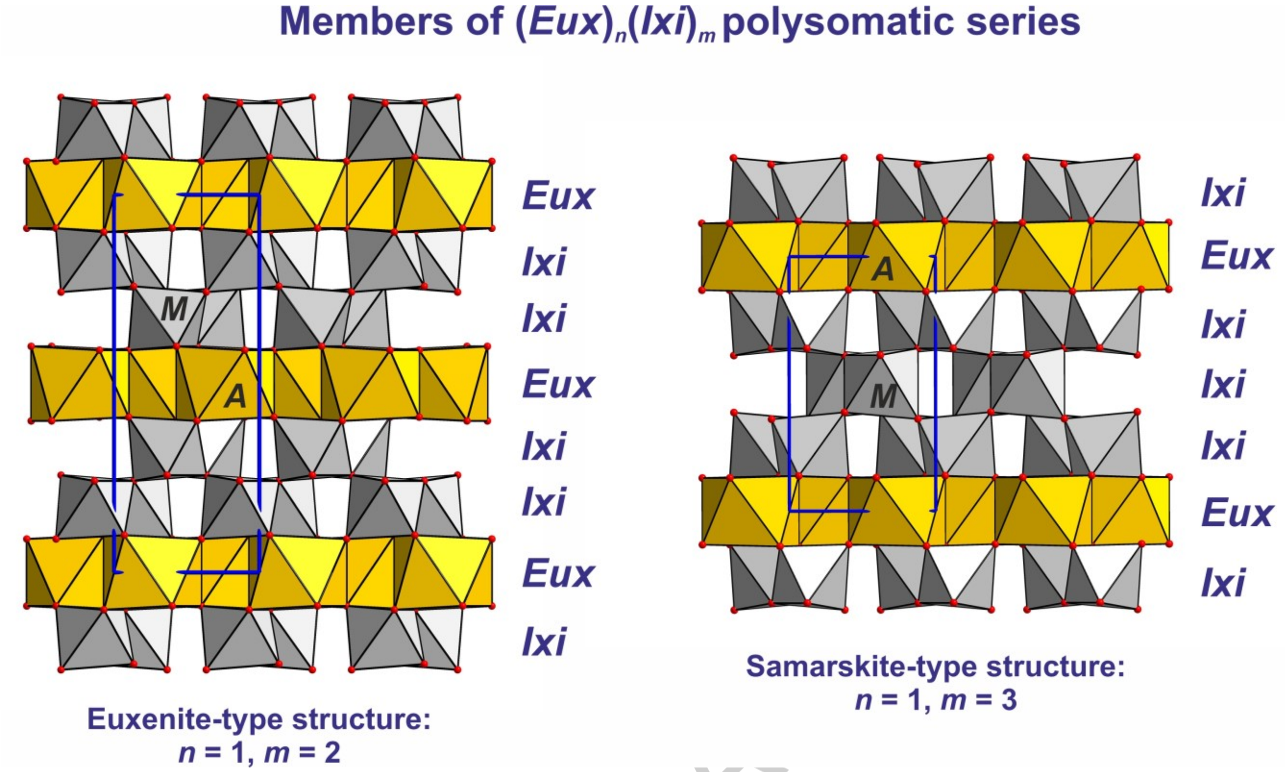


Fig. A1. Topological features of the ixiolite-type structures.



Euxenite-type structure: $n = 1$, $m = 2$

Samarskite-type structure: $n = 1$, $m = 3$

Fig. A2. The crystal structures of the members of $(Eux)_n(Ixi)_m$-polysomatic series.

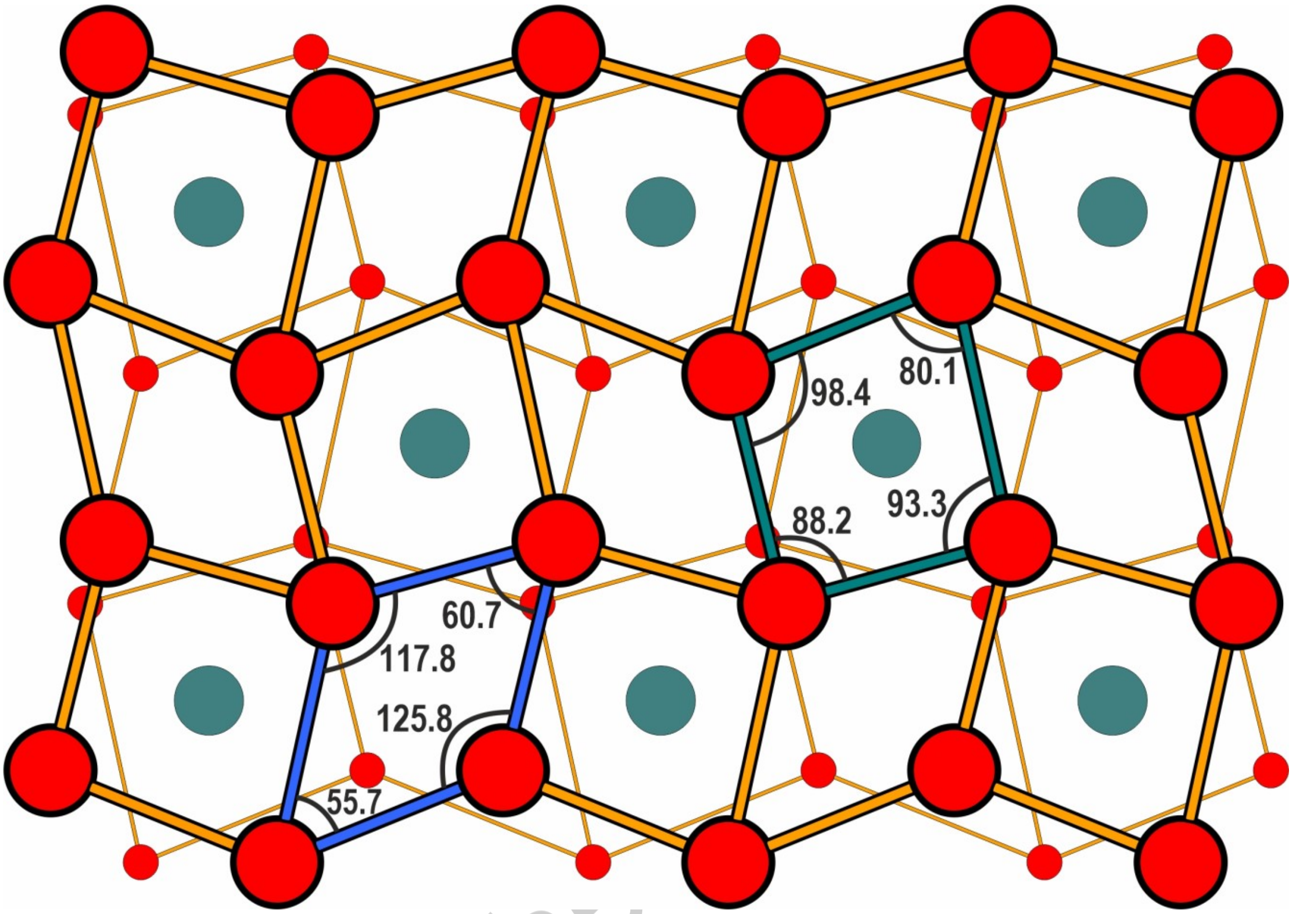


Fig. A3. The geometrical characteristics of the squares in the distorted *hcp* oxygen layers of *Eux*-module. Irregularity in the angles of the blue square in comparison with the greenish one, which forms the face of the AO_8-polyhedron, demonstrates the steric restriction of the direct linkage of two *Eux*-modules.

Table 1. Minerals belonging to the columbite supergroup.

Mineral species			Comments	References
Name	Endmember formula	Space group and unit-cell parameters		
Ixiolite group *M*O$_2$ **Orthorhombic *Pbcn*, $a = a_0$, $b = b_0$, $c = c_0$, $Z = 4$**				
Ixiolite-(Mn^{2+})	$(Ta_{2/3}Mn^{2+}_{1/3})O_2$	*Pbcn*, *a* 4.78, *b* 5.76, *c* 5.16 Å		Nordenskiöld, 1857; Grice *et al.*, 1976
Ixiolite-(Fe^{2+})	$(Ta_{2/3}Fe^{2+}_{1/3})O_2$	*Pbcn*, *a* 4.74, *b* 5.73, *c* 5.15 Å		Nordenskiöld, 1857; Nickel *et al.*, 1963a
Scrutinyite	α-PbO$_2$	*Pbcn*, *a* 4.97, *b* 5.66, *c* 5.44 Å		Zaslavskij and Tolkachev, 1952; Taggart *et al.*, 1988
Seifertite	SiO_2	*Pbcn*, *a* 4.10, *b* 5.05, *c* 4.49 Å		Dera *et al.*, 2002; El Goresy *et al.*, 2008; Zhang *et al.*, 2016
Srilankite	TiO_2	*Pbcn*, *a* 4.71, *b* 5.55, *c* 5.02 Å		Willgallis and Hartl, 1983; Chen *et al.*, 2013
Wolframite group *M*1*M*2O$_4$ **Monoclinic *P*2/*c*, $a = a_0$, $b = b_0$, $c = c_0$, $\beta \sim 91°$, $Z = 2$**				
Ferberite	$Fe^{2+}WO_4$	*P*2/*c*, *a* 4.75, *b* 5.72, *c* 4.97 Å, β 90.2°		Liebe, 1963; Escobar, 1968
Hübnerite	$Mn^{2+}WO_4$	*P*2/*c*, *a* 4.82, *b* 5.76, *c* 4.97 Å, β 89.1°		Credner, 1865; Dachs *et al.*, 1967
Huanzalaite	$MgWO_4$	*P*2/*c*, *a* 4.70, *b* 5.68, *c* 4.94 Å, β 90.8°		Miyawaki *et al.*, 2010
Sanmartinite	$ZnWO_4$	*P*2/*c*, *a* 4.69, *b* 5.73, *c* 4.92 Å, β 90.8°		Angelelli and Gordon, 1948; Redfern *et al.*, 1995
Heftetjernite	$ScTaO_4$	*P*2/*c*, *a* 4.78, *b* 5.69, *c* 5.12 Å, β 91.1°		Kolitsch *et al.*, 2010
Nioboheftetjernite	$ScNbO_4$	*P*2/*c*, *a* 4.71, *b* 5.65, *c* 5.05 Å, β 90.5°		Lykova *et al.*, 1921

Rossovskyite	$Fe^{3+}NbO_4$	*P*2/*c*, *a* 4.67, *b* 5.66, *c* 5.06 Å, β 90.2°		Konovalenko *et al.*, 2015
Riesite	$TiTiO_4$	*P*2/*b*, *a* 4.52, *b* 5.50, *c* 4.89 Å, β 90.6°		Tschauner *et al.*, 2020
Samarskite group *ABM*$_2$O$_8$ **Monoclinic *P2/c*, *a* = 2a$_0$, *b* = b$_0$, *c* = c$_0$, β ~ 93° *Z* = 2**				
Samarskite-(Y)	$YFe^{3+}Nb_2O_8$	*P*2/*c*, *a* 9.80, *b* 5.62, *c* 5.21 Å, β 93.4°		Britvin *et al.*, 2019
Ekebergite	$ThFe^{2+}Nb_2O_8$	*P*2/*c*, *a* 9.81, *b* 5.63, *c* 5.22 Å, β 93.5°	Isostructural with samarskite-(Y).	Kjellman *et al.*, 2018
Shakhdaraite-(Y)	$YScNb_2O_8$	*P*2/*c*, *a* 9.93, *b* 5.66, *c* 5.21 Å, β 92.4°	Isostructural with samarskite-(Y).	Pautov *et al.*, 2022
Samarskite-(Yb)	$YbFe^{3+}Nb_2O_8$ (?)	*a* 5.69, *b* 9.91, *c* 5.20 Å, β 93.2°	Metamict, the unit-cell parameters are questionable: compare samarskite-(Y).	Simmons *et al.*, 2006
Ishikawaite	$U^{4+}Fe^{2+}Nb_2O_8$	*a* 5.65, *b* 9.93, *c* 5.24 Å, β 93.9°	Metamict, the unit-cell parameters are questionable: compare samarskite-(Y).	Shimata and Kimura, 1922a,b; Hanson *et al.*, 1999.
Calciosamarskite	$CaFe^{3+}Nb_2O_7(OH)$	*a* 5.63, *b* 9.91, *c* 5.22 Å, β 93.9°	Questionable mineral: based on charge balance, the *A*-site in a hydrogen-free niobate with the samarskite-type structure cannot be M^{2+}-dominant.	Ellsworth, 1928a,b; Hanson *et al.*, 1999.
Columbite group *M*1*M*2$_2$O$_6$ **Orthorhombic *Pbcn*, *a* = 3a$_0$, *b* = b$_0$, *c* = c$_0$, *Z* = 4**				
Columbite-(Fe)	$Fe^{2+}Nb_2O_6$	*Pbcn*, *a* 14.24, *b* 5.73, *c* 5.09 Å		Jameson, 1805; Tarantino and Zema, 2005
Columbite-(Mn)	$Mn^{2+}Nb_2O_6$	*Pbcn*, *a* 14.32, *b* 5.74, *c* 5.11 Å		Dana, 1992; Tarantino and Zema, 2005
Columbite-(Mg)	$MgNb_2O_6$	*Pbcn*, *a* 14.19, *b* 5.70, *c* 5.03 Å		Mathias *et al.*, 1963; Pagola *et*

				al., 1997
Tantalite-(Fe)	$Fe^{2+}Ta_2O_6$	*Pbcn*, *a* 14.24, *b* 5.73, *c* 5.08 Å		Thomson, 1836; Ercit *et al.*, 1995
Tantalite-(Mn)	$Mn^{2+}Ta_2O_6$	*Pbcn*, *a* 14.41, *b* 5.76, *c* 5.08 Å		Nordenskiöld, 1877; Grice *et al.*, 1976
Tantalite-(Mg)	$MgTa_2O_6$	*Pbcn*, *a* 14.33, *b* 5.73, *c* 5.06 Å		Pekov *et al.*, 2003
Fersmite	$CaNb_2O_6$	*Pbcn*, *a* 14.93, *b* 5.75, *c* 5.20 Å (synthetic)		Aleksandrov, 1960; Gurbanova *et al.*, 2001
Euxenite-(Y)	$Y(NbTi)O_6$	*Pbcn*, *a* 14.64, *b* 5.55, *c* 5.20 Å (for synthetic $YNbTiO_6$)	Metamict. Presumed synthetic analogue is isostructural with columbite (Weitzel and Schröcke, 1980).	
Tanteuxenite-(Y)	$Y(TaTi)O_6$	*Pbcn*, *a* 14.57, *b* 5.56, *c* 5.18 Å	Metamict	
Uranopolycrase	UTi_2O_6	*Pbcn*, *a* 14.51, *b* 5.56, *c* 5.17 Å	Most natural samples are metamict. Isostructural with columbite (Aurisicchio *et al.*, 1993).	
Wodginite group $M1M2M3_2O_8$ **Monoclinic *C2/c*, $a = 2a_0$, $b = 2b_0$, $c = c_0$, $\beta \sim 91°$ $Z = 4$**				
Wodginite	$Mn^{2+}SnTa_2O_8$	*C2/c*, *a* 9.53, *b* 11.50, *c* 5.14 Å, β 91.2°		Nickel *et al.*, 1963a; Etcit *et al.*, 1992a
Ferrowodginite	$Fe^{2+}SnTa_2O_8$	*C2/c*, *a* 9.42, *b* 11.44, *c* 5.10 Å, β 90.8°		Ercit *et al.*, 1992c
Titanowodginite	$Mn^{2+}TiTa_2O_8$	*C2/c*, *a* 9.47, *b* 11.43, *c* 5.13 Å, β 90.3°		Ercit *et al.*, 1992c
Ferrotitanowodginite	$Fe^{2+}TiTa_2O_8$	*C2/c*, *a* 9.403, *b* 11.384, *c* 5.075 Å, β 90553°		Galliski *et al.*, 1999
Tantalowodginite	$(Mn_{0.5}\square_{0.5})TaTa_2O_8$	*C2/c*, *a* 9.542,		Hanson *et al.*,

		b 11.488, c 5.128 Å, β 91.13°		2018
Lithiowodginite	$LiTa_3O_8$	$C2/c$, a 9.44, b 11.52, c 5.06 Å, β 91.1°		Voloshin *et al.*, 1990
Achalaite	$Fe^{2+}TiNb_2O_8$	$C2/c$, a 9.422, b 11.427, c 5.120, β 90.12°		Galliski *et al.*, 2016
Ungrouped species				
Lithiotantite	$LiTa_3O_8$	$P2_1/c$, a 7.444, b 5.044, c 15.255 Å, β = 107.18°	Ixiolite-type topology. Related to lithiowodginite.	Voloshin *et al.*, 1990; Ercit *et al.*, 1992a,c
Other questionable, insufficiently studied minerals				
Qitianlingite	$Fe^{2+}_2Nb_2W^{6+}O_{10}$ (?)	$Pbcn$, a 23.71, b 5.72, c 5.04 Å (?)	Related to the columbite group? Needs further investigation.	Yang *et al.*, 1985; Peng *et al.*, 1988
Yttrocolumbite-(Y)	$YNbO_4$ (?)		Metamict. Related to the samarskite or wolframite group?	Lepierre, 1937
Yttrotantalite-(Y)	$YTaO_4$ (?)		Metamict. Related to the samarskite or wolframite group?	Ekeberg, 1802
Yttrocrasite-(Y)	$YTi_2O_5(OH)$ (?)		Metamict.	Palache *et al.*, 1944
"*Wolframixiolite*"	$(Nb_{2/3}Fe^{2+}_{1/3})O_2$ (?)	$P2/c$, a 4.750, b 5.72, c 5.06 Å, β = 90º (?)	Ixiolite group? Needs further investigation.	Ginzburg *et al.*, 1969; Borneman-Starynkevich *et al.*, 1974

Note: Names of insufficiently studied minerals are italicized.

Table 2. Changes in the formulae of columbite-supergroup minerals.

Mineral species	General formula	End-member formula
Ixiolite, now renamed ixiolite-(Mn^{2+})	$(Ta,Mn,Nb)O_2$	$(Ta_{2/3}Mn^{2+}_{1/3})O_2$
Srilankite	Ti_2ZrO_6	TiO_2
Rossovskyite	$(Fe^{3+},Ta)(Nb,Ti)O_4$	$Fe^{3+}NbO_4$
Fersmite	$(Ca,Ce,Na)(Nb,Ta,Ti)_2(O,OH,F)_6$	$CaNb_2O_6$
Euxenite-(Y)	$(Y,Ca,Ce,U,Th)(Nb,Ta,Ti)_2O_6$	$Y(NbTi)O_6$
Tanteuxenite-(Y)	$Y(Ta,Nb,Ti)_2(O,OH)_6$	$Y(TaTi)O_6$

Uranopolycrase	(U,Y)(Ti,Nb,Ta)$_2$(O,OH)$_6$	UTi$_2$O$_6$