OXIDES

- CLASS D OXIDES
- GROUP A COORDINATION STRUCTURE

TYPE A SIMPLE

SERIES A FLUORITE STRUCTURE, CN = 8/4, cub/Fm3m. The fluorite structure is based on a simple cubic packing of the F atoms, with Ca occupying 1/2 of the cubic voids, forming a square pattern.

DAAAA	THORIANITE	ThO ₂
DAAAB	CERIANITE-(Ce)	(Ce,Th)O ₂
DAAAC	URANINITE	UO ₂
DAAAD	VORLANITE	(CaU ⁶⁺)O ₄

SERIES B BADDELEYITE SERIES, CN = 7, mon/P2₁/c. Structure consists of a framework of edge- and cornersharing ZrO₇ polyhedra.

DAABA	BADDELEYITE	ZrO_2
DAABB	TUGARINOVITE	MoO ₂
DAABC	AKAOGIITE	TiO ₂
DAABD	RIESITE	TiO ₂

SERIES C CORUNDUM SERIES, CN = 7, trig/R3c. Structure consists of a lattice of hexagonal closed-packed O atoms in which 2/3 of the octahedral sites are occupied by trivalent cations. The octahedra share edges to form 6-membered rings, and these are lined into gibbsite-like sheets // (0001). The sheets are linked into a framework by sharing faces and corners of octahedra.

DAACA	CORUNDUM	AI_2O_3	
DAACB	HEMATITE	Fe_2O_3	
DAACC	ESKOLAITE	Cr_2O_3	
DAACD	TISTARITE	Ti_2O_3	
DAACE	KARELIANITE	V_2O_3	
DAACF	LUOGUFENGITE	Fe_2O_3	orth/Pna21
DAACG	DELTALUMITE	AI_2O_3	

SERIES D BIXBYITE SERIES, CN = 6/4, cub/la3. Structure consists of M octahedra sharing edges to form undulating chains along the principal crystal axes; the chains are linked into a checkerboard-like framework by sharing corners.

DAADA	BIXBYITE	Mn ₂ O ₃
DAADB	AVICENNITE	TI_2O_3
DAADC	MAGHEMITE	Fe ₂ O ₃
DAADD	YTTRIAITE-(Y)	Y_2O_3
DAADE	KANGITE	(Sc,Ti,Al,Zr,Mg,Ca) ₂ O ₃
DAADF	PANGUITE	(Ti,AI,Sc,Mg,Zr,Ca) _{1.8} O ₃
DAADG	MCALPINEITE	Cu ₃ TeO ₆ cub/la <u>3</u>

Roberts, A. C., Ercit, T. S., & Cureton, F. F. (1994). Mcalpineite, Cu3TeO6. H20, from the McAlpine mine, Tuolumne County, California, and from the Centennial Eureka mine, Juab County, Utah I. Mineralogical Magazine, 58, 417-424.

Carbone, C., Basso, R., Cabella, R., Martinelli, A., Grice, J.D. and Lucchetti, G. (2013) Mcalpineite from the Gambatesa mine, Italy, and redefinition of the species. American Mineralogist, 98, 1899-1905. Isostructural with bixbyite.

SERIES E BISMITE, mon/P2₁/c. Structure consists of irregular BiO_6 polyhedra sharing corners and edges to form a framework. In sillenite, BiO_4 tetrahedra and flat BiO_3 pyramids share corners to form a framework. Some vacant O sites in the lattice create BiO_3 umbrella-shaped polyhedra.

DAAEA	BISMITE	Bi_2O_3
DAAEB	SPHAEROBISMOITE	Bi_2O_3
DAAEC	SILLENITE	$Bi_{12}SiO_{20}$

SERIES F HALITE Structure SERIES, CN = 6/6, cub/Fm3m. The structure is formed by the closest packing of Cl⁻ anions in cubic closest packing with Na⁺ cations occupying all the octahedral interstices.

DAAFA	PARICLASE	MgO
DAAFB	BUNSENITE	NiO
DAAFC	MANGANOSITE	MnO
DAAFD	LIME	CaO
DAAFE	WÜSTITE	Fe _{1-x} O
DAAFF	MONTEPONITE	CdO
DAAFG	MURDOCHITE	$Cu_6PbO_{8-x}(CI,Br)_{2x} x = .5$ (defect halite structure) cub/Fm3m
DAAFH	EDDAVIDITE	$Pb_2Cu_{12}O_{15}Br_2$

SERIES G WÜRTZITE Structure SERIES, CN = 4/4, hex/P6₃mc. Structure based on a hexagonal closest packing of the S atoms, with Zn atoms occupying one half of the tetrahedral voids, resulting in a triangular distribution pattern.

DAAGA	ZINCITE	ZnO
DAAGB	BROMELLITE	BeO

SERIES H TENORITE, mon/C2/c. The structure is a distortion derivative of cooperite. It is based on a simple cubic packing of the O atoms, with Cu atoms occupying 1/2 of the square voids. Structure consists of CuO₄ square planes sharing edges to form chains // [110] and [<u>1</u>10]; the chains are linked by sharing corners.

DAAHA TENORITE CuO mon/C2/c

SERIES I Open

SERIES J CUPRITE, cub/Pn3m. The structure consists of a framework of O^tCu₄ tetrahedra in a ball and spoke configuration. The structure of paramelaconite is closely related to cuprite and tenorite and consists of interpenetrating rods of Cu-O (Cu⁺ forming two co-linear bonds with oxygen) and Cu²⁺-O (Cu²⁺ forming four bonds to oxygen atoms at the corners of a rectangle).

DAAJA	CUPRITE	Cu ₂ O	
DAAJB	PARAMELACONITE	$Cu_2^{1+}Cu_2^{2+}O_3$	tetr/I4 ₁ /amd AM63-184
DAAJC	ICE-VII	H ₂ O	

SERIES K ALLENDEITE, trig/R3. Allendeite has a fluorite-related superstructure. Zr and Sc are both sevencoordinated to oxygen.

DAAKA ALLENDEITE Sc₄Zr₃O₁₂

TYPE B COMPLEX

SERIES A SCHEELITE Structure SERIES, CN = 8, tetr/I4₁/a. The scheelite structure is a non-layered structure, and is formed by isolated WO₄ tetrahedra separated by Ca atoms, each of which is bonded to 8 oxygen atoms forming a dodecahedron. This structure is a distortion derivative of the zircon structure.

DABAA	FERGUSONITE-(Ce)	(Ce,La,Y)NbO ₄
DABAB	FERGUSONITE-(Nd)	(Nd,Ce)(Nb,Ti)O ₄
DABAC	FERGUSONITE-(Y)	YNbO ₄
DABAD	FORMANITE-(Y)	YTaO₄

SERIES B FERGUSONITE-BETA SERIES, CN = 8, mon/l2. The structure is closely related to the alpha-PbO₂ and fluorite structures. Structures consist of TaO₆ octahedra and YO₈ polyhedra.

DABBA	FERGUSONITE-BETA-(Ce)	(Ce,La,Nd)NbO ₄	
DABBB	FERGUSONITE-BETA-(Nd)	(Nd,Ce,La)NbO ₄	
DABBC	FERGUSONITE-BETA-(Y)	YNbO ₄	
DABBD	YTTROCOLUMBITE-(Y)	(Y,U,Fe)(Nb,Ta)O ₄	
DABBE	YTTROTANTALITE-(Y)	(Y,U,Fe)(Ta,Nb)O ₄	
DABBF	ISHIKAWAITE	(U,Fe,Y,Ca)(Nb,Ta)O ₄	orth/
DABBG	IWASHIROITE-(Y)	YTaO ₄	mon/P2/a
DABBH	TAKANAWAITE-(Y)	YtaO ₄	mon/I2/a

SERIES C STIBIOCOLUMBITE Structure SERIES, CN = 6, orth/Pc21n. The structure is built up of slices of the ReO₃ structure parallel to (100) and has Sb atoms sandwiched in between to form two closely related structures both of which are very similar to thoreaulite. In the crystal structure of kyawthuite (R1 = 0.0269 for 593 reflections with Fo > 4\sigmaF), Sb5+O6 octahedra share corners to form checkerboard-like sheets parallel to {001}. Bi3+ atoms, located above and below the open squares in the sheets, form bonds to the O atoms in the sheets, thereby linking adjacent sheets into a framework. Bi3+ is in lopsided 8 coordination, typical of a cation with stereoactive lone electron pairs. Kyawthuite is isostructural with synthetic β -Sb2O4 and clinocervantite (natural β -Sb2O4).

DABCA	STIBIOCOLUMBITE	SbNbO ₄
DABCB	STIBIOTANTALITE	SbTaO ₄
DABCC	BISMUTOTANATALITE	Bi(Ta,Nb)O ₄
DABCD	ALUMOTANTALITE	AITaO ₄
DABCE	CERVANTITE	SbSbO ₄
DABCF	BISMUTOCOLUMBITE	Bi(Nb,Ta)O ₄
DABCG	CLINOCERVANTITE	$Sb_2O_4(Sb^{3+}Sb^{5+}O_4)$ monoclinic polymorph of cervantite
DABCH	KYAWTHUITE	Bi ³⁺ Sb ⁵⁺ O ₄

SERIES D PYROCHLORE SERIES, cub/Fd3m. (Niobium-dominant) The structure is based on a defect simple cubic packing of the OH and O atoms, with Na, Ca, and Nb occupying 1/2 of the cubic voids. The large cations Na and Ca have cubic coordination, while Nb has 6 coordination, due to the vacancies in the structure. Structure consists of corner-sharing (Nb,Ta,Ti)O₆ octahedra forming sheets of 3- and 6-membered rings // {110} with channels in the <110> directions that accommodates the (Na,Ca) atoms. PHYLLOTUNGSTITE, orth/Cmcm. Structure of phyllotungstite can be described in terms of an ordered intergrowth to (001), of (111) blocks with pyrochlore-type structures and two-layer wide regions with a hexagonal tungsten bronze type structure. Cs atoms occupy 18 coordinate cavites in the HTB regions, and water molecules occupy F sites in the A₂B₂O₆F pyrochlore blocks. Hydroxynatropyrochlore, (Na,Ca,Ce)2Nb2O6(OH), is a new Na-Nb-OH-dominant member of the pyrochlore supergroup from the Kovdor phoscorite-carbonatite pipe (Kola Peninsula, Russia). It is cubic, Fd-3m, a = 10.3211(3) Å, V = 1099.46 (8) Å3, Z = 8 (from powder diffraction data) or a = 10.3276(5) Å, V = 1101.5(2) Å3, Z = 8 (from single-crystal diffraction data). Hydroxynatropyrochlore is

a characteristic accessory mineral of low-carbonate phoscorite of the contact zone of the phoscorite-carbonatite pipe with host foidolite as well as of carbonate-rich phoscorite and carbonatite of the pipe axial zone. It usually forms zonal cubic or cubooctahedral crystals (up to 0.5 mm in diameter) with irregularly shaped relics of amorphous U-Ta-rich hydroxykenopyrochlore inside. Characteristic associated minerals include rock-forming calcite, dolomite, forsterite, hydroxylapatite, magnetite, and phlogopite, accessory baddeleyite, baryte, barytocalcite, chalcopyrite, chamosite-clinochlore, galena, gladiusite, juonniite, ilmenite, magnesite, pyrite, pyrrhotite, quintinite, spinel, strontianite, valleriite, and zirconolite. Hydroxynatropyrochlore is palebrown, with an adamantine to greasy lustre and a white streak. The cleavage is average on {111}, the fracture is conchoidal. Mohs hardness is about 5. In transmitted light, the mineral is light brown, isotropic, n = 2.10(5) (delta = 589 nm). The calculated and measured densities are 4.77 and 4.60(5) q-cm-3, respectively. The mean chemical composition determined by electron microprobe is: F 0.05, Na2O 7.97, CaO 10.38, TiO2 4.71, FeO 0.42, Nb2O5 56.44, Ce2O3 3.56, Ta2O5 4.73, ThO2 5.73, UO2 3.66, total 97.65 wt. %. The empirical formula calculated on the basis of Nb+Ta+Ti = 2 apfu is (Na1.02Ca0.73Ce0.09Th0.09 U0.05Fe2+0.02)Σ2.00 (Nb1.68Ti0.23Ta0.09) 22.0006.03 (OH1.04F0.01) 21.05. The simplified formula is (Na, Ca,Ce)2Nb2O6(OH). The mineral slowly dissolves in hot HCI. The strongest X-ray powder-diffraction lines [listed as (d in Å)(l)(hkl)] are as follows: 5.96(47)(111), 3.110(30)(311), 2.580(100)(222), 2.368(19)(400), 1.9875(6)(333), 1.8257(25)(440) and 1.5561(14)(622). The crystal structure of hydroxynatropyrochlore was refined to R1 = 0.026 on the basis of 1819 unique observed reflections.

The mineral belongs to the pyrochlore structure type A2B2O6Y1 with octahedral framework of corner-sharing BO6 octahedra with A cations and OH groups in the interstices. The Raman spectrum of hydroxynatropyrochlore contains characteristic bands of the lattice, BO6, B–O and O–H vibrations and no characteristic bands of the H2O vibrations. Within the Kovdor phoscorite-carbonatite pipe, hydroxynatropyrochlore is the latest hydrothermal mineral of the pyrochlore supergroup, which forms external rims around grains of earlier U-rich hydroxykenopyrochlore and separated crystals in voids of dolomite carbonatite veins. The mineral is named in accordance with the pyrochlore supergroup nomenclature.

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- DABDA OXYCALCIOPYROCHLORE
- DABDB HYDROPYROCHLORE
- DABDC HYDROXYCALCIOPYROCHLORE
- DABDD OXYYTTROPYROCHLORE-(Y)
- DABDE FLUORCALCIOPYROCHLORE
- DABDF OXYPLUMBOPYROCHLORE
- DABDG KENOPLUMBOPYROCHLORE
- DABDH FLUORNATROPYROCHLORE
- DABDI OXYNATROPYROCHLORE

 $Ca_{2}Nb_{2}O_{6}$ $(H_{2}O, \Box)_{2}Nb_{2}(O,OH)_{6}(H_{2}O)$ $(Ca, \Box)_{2}Nb_{2}(O,OH)_{6}(OH)$ $(Y, \Box)_{2}Nb_{2}O_{6}O$ $(Ca, \Box)_{2}Nb_{2}(O,OH)_{6}F$ $Pb_{2}Nb_{2}O_{6}O$ $(Pb, \Box)_{2}Nb_{2}O_{6}(\Box,O)$ $(Na,REE,Ca)_{2}Nb_{2}(O,OH)_{6}F$ $(Na,Ca,U)_{2}Nb_{2}O_{6}(O,OH)$

DABDJ	FLUORSTRONTIOPYROCHLORE	(Sr,□) ₂ Nb ₂ (O,OH) ₆ F
DABDK	FLUORKENOPYROCHLORE	(□,Na,Ce,Ca)₂(Nb,Ti)₂O ₆ F
DABDL	ZERO-VALENT-DOMINANT PYROCHLORE	No definite chemistry
DABDM	TAZZOLIITE	$Ba_{4} \Box_{x} Na_{x} Ti_{2} Nb_{3} SiO_{17} [PO_{2}(OH)_{2}]_{x} (OH)(1 \Box_{2x})(04_{x} 40.5)$
DABDN	HYDROXYMANGANOPYROCHLORE	(Mn,Th,Na,Ca,REE) ₂ (Nb,Ti) ₂ O ₆ (OH)
DABNO	FLUORNATROPYROCHLORE	(Na,Pb,Ca,REE,U) ₂ Nb ₂ O ₆ F
DABNP	FLUORCALCIOPYROCHLORE	(Ca,Na) ₂ (Nb,Ti) ₂ O ₆ F
DABNQ	PHYLLOTUNGSTITE, orth/Cmcm	$Cs_{0.41}(Na,K,Pb,Ca[W_{10.87}Fe_{3.13}O_{35.75}(OH)_{6.25}]O(H_2O)_3$
DABNR	HYDROXYFERROROMEITE	(Fe ²⁺ _{1.5} □ _{0.5})Sb ⁵⁺ ₂ O ₆ (OH)
DABNS	FLUORNATROCOULSELLITE	CaNa ₃ AIMg ₃ F ₁₄ Rom/R <u>3</u> m
DABNT	CESIOKENOPYROCHLORE	□Nb ₂ (O,OH) ₆ Cs _{1-x} (x ~ 0.020)
DABNU	HYDROKENOPYROCHLORE	$\Box_2 Nb_2 O_4 (OH)_2 (H_2 O)$
DABNV	HYDROXYKENOPYROCHLORE	(□,Ce,Ba)₂(Nb,Ti)₂O ₆ (OH,F)
DABNW	HYDROXYNATROPYROCHLORE	(Na,Ca,Ce) ₂ Nb ₂ O ₆ (OH)

SERIES E	MICROLITE SERIES. (Tantalum-dominant)	
DABEA	FLUORNATROMICROLITE	(Na,Ca,Bi) ₂ Ta ₂ O ₆ F
DABEB	HYDROXYKENOMICROLITE	(□,Na,Sb ³⁺)₂Ta₂O ₆ (OH)
DABEC	HYDROKENOMICROLITE-3R	(□,H ₂ O) ₂ Ta ₂ (O,OH) ₆ (H ₂ O)
DABED	FLUORCALCIOMICROLITE	(Ca,Na) ₂ Ta ₂ O ₆ F
DABEE	OXYCALCIOMICROLITE	$Ca_2Ta_2O_6O$
DABEF	KENOPLUMBOMICROLITE	(Pb,□) ₂ Ta ₂ O ₆ (□,O,OH)
DABEG	OXYSTANNOMICROLITE	Sn ₂ Ta ₂ O ₆ O
DABEH	OXYSTIBIOMICROLITE	(Sb ³⁺ ,Ca) ₂ Ta ₂ O ₆ O
DABEI	HYDROMICROLITE	$(H_2O,\Box)_2Ta_2(O,OH)_6(H_2O)$
DABEJ	ZERO-VALENT-DOMINANT MICROLITE	No definite chemistry
DABEK	open	
DABEL	OXYNATROMICROLITE	(Na,Ca,U) ₂ (Ta,Nb) ₂ O ₆ (O,F)
DABEM	HYDROXYCALCIOMICROLITE	Ca _{1.5} Ta ₂ O ₆ (OH)

SERIES F BETAFITE SERIES. (Titanium-dominant). Laachite is the Ti member of zirconolite structure type.

DABFA	OXYCALCIOBETAFITE	Ca ₂ (Ti,Nb) ₂ O ₆ O
DABFB	OXYURANOBETAFITE	(U,Ca,□)₂(Ti,Nb)₂O ₆ O
DABFC	open	
DABFD	open	
DABFE	LAACHITE	(Ca,Mn) ₂ (Zr,Mn) ₂ Nb ₂ TiFeO ₂₄ mon/C2/c
DABFF	ZIRKELITE	(Ca,Th,Ce)Zr(Ti,Nb) ₂ O ₇ P3 ₁ 2
DABFG	NOGGERATHITE-(Ce)	(Ce,Ca) ₂ Zr ₂ (Nb,Ti)(Ti,Nb) ₂ Fe ²⁺ O ₁₄ orth/Cmca
DABFH	ZIRCONOLITE, 30, 3T	CaZrTi ₂ O ₇ mon/C2/c
DABFI	STEFANWEISSITE	(Ca,REE) ₂ Zr ₂ (NbkTi)(Ti,Nb) ₂ Fe ²⁺ O ₁₄

SERIES G ELSMOREITE SERIES. (Tungsten-dominant)

DABGA HYDROKENOELSMOREITE

 $\square_2W_2O_6(H_2O)$

DABGB HYDROXYKENOELSMOREITE

 $(\Box, Pb)_2(W, Fe, AI)_2(O, OH)_6(OH)$

SERIES H	ROMEITE SERIES. (Antimony-dominant)	
DABHA	STIBIOROMEITE	SbSb ₂ O ₆ (OH)
DABHB	ARGENTOROMEITE	Ag ₂ Sb ₂ (O,OH) ₇
DABHC	OXYCALCIOROMEITE	$Ca_2Sb_2O_6O$
DABHD	OXYPLUMBOROMEITE	$Pb_2Sb_2O_6O$
DABHE	BISMUTOROMEITE	Bi(Sb,Fe) ₂ O ₇
DABHF	INGERSONITE	Ca ₃ MnSb ₄ O ₁₄ , hex/P3 ₁ 21 (Structure in AM07-947)
DABHG	CUPROROMEITE	Cu ₂ Sb(O,OH) ₇
DABHH	HYDROXYCALCIOROMEITE	(Ca,Sb ³⁺) ₂ (Sb ⁵⁺ ,Ti) ₂ O ₆ (OH)
DABHI	FLUORNATROROMEITE	(Na,Ca) ₂ Sb ₂ (O,OH) ₆ F
DABHJ	FLUORCALCIOROMEITE	(Ca,Sb ³⁺) ₂ (Sb ⁵⁺ ,Ti) ₂ O ₆ F

SERIES I CORUNDUM Derivative Structures, CN = 6/4, trig/R<u>3</u>. The structure is an interstitial substitution derivative of corundum. The oxygen atoms form an hexagonal closest packing and Fe and Ti occupy 2/3 of the octahedral voids, with a honeycomb pattern, in alternate layers.

DABIA	ILMENITE	FeTiO ₃	
DABIB	PYROPHANITE	MnTiO ₃	
DABIC	GEIKIELITE	MgTiO ₃	
DABID	ECANDREWSITE	$(Zr,Fe,Mn)TiO_3$	
DABIE	BRIZZIITE	NaSbO₃	
DABIF	PSEUDORUTILE	Fe ₂ Ti ₃ O ₉	P322
DABIG	MELANOSTIBITE	Mn(Sb,Fe)O₃	
DABIH	New mineral name	FeCrO ₃	
DABIJ	PAULOABIBITE	NaNbO₃	trig/R3
DABIK	WANGDAODEITE	FeTiO ₃	trig/R3c
DABIL	HEMLEYITE	FeSiO ₃	
DABIM	LIUITE	FeTiO ₃	orth/Pnma

SERIES J MAGNETOPLUMBITE, trig/P6₃/mmc. The structure comprises alternating spinel-type slabs and perovskite-type layers.

DABJA	MAGNETOPLUMBITE	Pb(Fe,Mn) ₁₂ O ₁₉
DABJB	HAWTHORNEITE	Ba(Ti ₃ Cr ₄ Fe ₂ Mg)O ₁₉
DABJC	HIBONITE	(Ca,Ce)(AI,Ti,Mg) ₁₂ O ₁₉
DABJD	YIMENGITE	K(Cr,Ti,Fe,Mg) ₁₂ O ₁₉
DABJE	LINDQVISTITE	Pb ₂ (Mg,Fe)Fe ₁₆ O ₂₇
DABJF	PLUMBOFERRITE	PbFe ₄ O ₇ , trig/P312
DABJG	NEZILOVITE	PbZn ₂ (Mn ⁴⁺ ,Ti ⁴⁺) ₂ Fe ₈ O ₁₉
DABJH	HAGGERTYITE	Ba[Fe ₆ Ti₅Mg]O ₁₉
DABJI	BATIFERRITE	Ba[Ti ₂ Fe ³⁺ 8Fe ² 2]O ₁₉
DABJJ	OTJISUMEITE	PbO[Ge ₄ O ₈]
DABJK	HIBONITE-(Fe)	(Fe,Mg)AI ₁₂ O ₁₉
DABJL	BARIOFERRITE	BaFe ³⁺ 12O19

SERIES K CRICHTONITE, trig-mon/R<u>3</u>. The structure is based on a close-packed anion framework with a ninelayer stacking sequence in which Sr, REE, and Pb atoms occupy one of the anionic sites in the cubic layers. The other metal atoms are ordered into both tetrahedral and octahedral interstices between the anion layers.

DABKA	CRICHTONITE	(Sr,La,Ce,Y)(Ti,Fe,Mn) ₂₁ O ₃₈
DABKB	DAVIDITE-(Ce)	(Ce,La)(Y,U,Fe)(Ti,Fe) ₂₀ (O,OH) ₃₈
DABKC	DAVIDITE-(La)	(La,Ce)(Y,U,Fe)(Ti,Fe) ₂₀ (O,OH) ₃₈
DABKD	LANDAUITE	NaMnZn ₂ (Ti,Fe) ₆ Ti ₁₂ O ₃₈
DABKE	LINDSLEYITE	BaMn ₃ Ti ₁₄ ⁴⁺ Ti ₄ ³⁺ O ₃₈
DABKF	LOVERINGITE	(Ca,Ce)(Ti,Fe,Cr,Mg) ₂₁ O ₃₈
DABKG	MATHIASITE	(K,Ca,Sr)(Ti,Cr,Fe,Mg) ₂₁ O ₃₈
DABKH	SENAITE	Pb(Ti,Fe,Mn) ₂₁ O ₃₈
DABKI	MURATAITE-(Y)	$(Na,Y)_{6}(Zn,Fe)_{5}(Ti,Nb)_{12}O_{29}(O,F)_{10}F_{4}, cub/F_{4}3m$
DABKJ	DESSAUITE-(Y)	(Sr,Pb)(Y,U)(Ti,Fe) ₂₀ O ₃₈ trig/R <u>3</u>
DABKL	GRAMACCIOLIITE-(Y)	(Pb,Sr)(Y,Mn)Fe ₂ (Ti,Fe) ₁₈ O ₃₈
DABKM	CLEUSONITE	Pb(U ⁴⁺ ,U ⁶⁺))(Ti,Fe ²⁺ Fe ³⁺) ₂₀ (O,OH) ₃₈
DABKN	PASEROITE	PbMn ²⁺ (Fe,□) ₂ (V ⁵⁺ ,Ti,□) ₁₈ O ₃₈
DABKO	MAPIQUIROITE	(Sr,Pb)(Y,Y)Fe ₂ (Ti,Fe,Cr) ₁₈ O ₃₈
DABKP	ALMEIDAITE	PbZn ₂ (Mn,Y)(Ti,Fe) ₁₈ O ₃₆ (OH,O) ₂
DABKQ	MIANNINGITE	(&,Pb,Ce,Na)(U ⁴⁺ ,Mn,U ⁶⁺)Fe ³⁺ ₂ (Ti,Fe ³⁺) ₁₈ O ₃₈

SERIES L SPINEL/NOLANITE-LIKE Structures, hex/P6₃mmc. The model is based on a close packed anion framework with a 24 layer mixed stacking sequence along c. The interlayer articulation of the various polyhedra is controlled by the oxygen stacking sequence and is such that tetrahedra share only corners with octahedra, and octahedra share edges and corners.

DABLA	MAGNESIOHÖGBOMITE-2N2S	(Mg,Al,Fe,Ti) ₂₂ O ₃₀ (OH) ₂
DABLB	MAGNESIOHÖGBOMITE-2N3S	(Mg,Al,Fe,Ti) _{9.6} O ₃₈ (OH) ₂
DABLC	MAGNESIOHÖGBOMITE-6N6S	(Mg,Al,Fe,Ti) ₆₆ (O,OH) ₉₆
DABLD	ZINCOHÖGBÖMITE-2N2S	(Zn,Al,Fe,Ti) ₂₂ (O,OH) ₃₂
DABLE	ZINCOHÖGBOMITE-2N6S	(Zn,Fe,Ni,Mg,Co,Ti)Al₄O ₈
DABLF	FERRONIGERITE-2N1S	Al _{10.9} Sn ₂ Fe _{1.7} O ₂₂ (OH) ₂
DABLG	FERRONIGERITE-6N6S	AI _{10.9} Sn ₂ Fe _{1.7} O ₂₂ (OH) ₂
DABLH	MAGNESIONIGERITE-2N1S	$(Mg,AI,Zn)_4(Sn,Fe)_2AI_{10}O_{22}(OH)_2$
DABLI	MAGNESIONIGERITE-6N6S	(Mg,Al,Fe,Ti) ₂₂ O ₃₀ (OH) ₂
DABLJ	MAGNESIOTAAFFEITE-2N'2S	Mg ₃ BeAl ₈ O ₁₆
DABLK	MAGNESIOTAAFFEITE-6N'3S	$(Mg,Fe,Zn)_2BeAI_6O_{12}$
DABLL	FERROTAAFFEITE-6N'3S	Be(Fe,Zn,Mg) ₂ Al ₆ O ₁₂
DABLM	FERROHÖGBOMITE-2N2S	(Fe, Mg,AI,Ti) ₂₂ O ₃₀ (OH) ₂
DABLN	FERROTAAFFEITE-2N'2S	Be(Fe,Mg,Zn) ₃ Al ₈ O ₁₆
DABLO	MAGNESIOHÖGBOMITE-2N4S	(Mg,AI,Fe,Ti) _{9.6} O ₃₈ (OH)
DABLP	MAGNESIOBELTRANDOITE-2N3	S (Mg ₆ Al ₂)(Al ₁₈ Fe ³⁺ ₂)O ₃₈ (OH) ₂
DABLQ	ZINCOVELESITE-6N6S	Zn ₃ (Fe ³⁺ Mn ³⁺ Al,Ti) ₈ O ₁₅ (OH)
DABLR	ZINCONIGERITE-2N1S	$ZnSn_2AI_{12}O_{22}(OH)_2$

SERIES M NOLANITE, trig/P6₃mc. Nolanite is isostructural with the M₂Mo₃O₈ group of synthetic compounds. It is based on a closest-packed anion framework with hc stacking and with cations ordered into six-fold and two-fold octahedral sites and into a two-fold tetrahedral site. Two types of cation (001) layers alternate in nolanite; the six-fold sites form a layer of edge-shared octahedra identical with the (111) octahedral layers in spinel and the two-fold sites form a layer of corner-shared octahedra and tetrahedra. The two-fold octahedrally coordinated M(2) shares corners with a six-membered ring of M(1) octahedra in one layer and shares edges with a triangular cluster of M(1) octahedra in the opposite layer. The structure of iseite is based on the kamiokite-type structure. The MoO₄ tetrahedra and MnO₆ octahedra are connected at the apical oxygen atoms to form a honeycomb-like lattice sheets in the a-b plane those sheets stack with the Mo octahedral sheet alternately along the c-axis.

DABMA	NOLANITE	(V,Fe,Fe,Ti) ₁₀ O ₁₄ (OH) ₂	
DABMB	RINMANITE	$Zn_2Mg_2Fe_4Sb_2O_{14}(OH)_2$	
DABMC	KAMIOKITE	Fe ₂ Mo ₃ O ₈	hex/P6₃mc
DABMD	ISEITE	$Mn_2Mo_3O_8$	hex/P6₃mc
DABME	MAJINDEITE	Mg ₂ Mo ₃ O ₈	hex/P6₃mc

SERIES N OLIVINE Structure type, orth/Pmab. Structure based on zigzag chains of edge-sharing octahedra cross-linked by Si tetrahedra sharing three edges with the octahedra.

DABNA	CHRYSOBERYL	BeAl ₂ O ₄
DABNB	MAROKITE	$CaMn_2O_4$
DABNC	MARIINSKITE	$BeCr_2O_4$

SERIES O SPINEL SERIES, cub/Fd3m. The structure is based on a cubic closest packing of oxygen atoms with a half of the octahedral voids occupied by AI atoms forming a T lattice complex, and 1/8 of the tetrahedral voids occupied by Mg atoms forming a F lattice complex. Maohokite, a post-spinel polymorph of MgFe2O4, was found in shocked gneiss from the Xiuyan crater in China. Maohokite in shocked gneiss coexists with diamond, reidite, TiO2-II, as well as diaplectic glasses of guartz and feldspar. Maohokite occurs as nano-sized crystallites. The empirical formula is (Mg0.62Fe0.35Mn0.03)2+Fe3+2O4. In situ synchrotron X-ray microdiffraction established maohokite to be orthorhombic with the CaFe2O4-type structure. The cell parameters are a = 8.907 (1) A, b = 9.937(8) A, c = 2.981 (1) A; V = 263.8 (3) A3; space group Pnma. The calculated density of machokite is 5.33 g cm3. Machokite was formed from subsolidus decomposition of ankerite Ca(Fe2+,Mg)(CO3)2 via a self-oxidation-reduction reaction at impact pressure and temperature of 25-45 GPa and 800-900 °C. The formation of maohokite provides a unique example for decomposition of Fe-Mg carbonate under shock-induced high pressure and high temperature. The mineral and its name have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA 2017-047). The mineral was named maohokite after Hokwang Mao, a staff scientist at the Geophysical Laboratory,

DABOA	SPINEL	$MgAl_2O_4$
DABOB	GALAXITE	$MnAl_2O_4$
DABOC	HERCYNITE	FeAl ₂ O ₄
DABOD	GAHNITE	$ZnAl_2O_4$
DABOE	MAGNETITE	FeFe ₂ O ₄
DABOF	MAGNESIOFERRITE	$MgFe_2O_4$
DABOG	JACOBSITE	$MnFe_2O_4$
DABOH	FRANKLINITE	$ZnFe_2O_4$
DABOI	TREVORITE	NiFe ₂ O ₄
DABOJ	CUPROSPINEL	CuFe ₂ O ₄
DABOK	BRUNOGEIERITE	GeFe ₂ O ₄
DABOL	MAGNESIOCHROMITE	MgCr ₂ O ₄
DABOM	MANGANOCHROMITE	$(Mn,Fe)Cr_2O_4$

CHROMITE	FeCr ₂ O ₄	
NICHROMITE	(Ni,Co)(Cr,Fe) ₂ O ₄	
COCHROMITE	(Co,Ni)(Cr,Al) ₂ O ₄	
ZINCOCHROMITE	ZnCr ₂ O ₄	
COULSONITE	FeV ₂ O ₄	
VUORELAINENITE	(Mn,Fe)(V,Cr) ₂ O ₄	
ULVÖSPINEL	Fe ₂ TiO ₄	
QANDILITE	(Mg,Fe) ₂ (Ti,Fe,Al)O ₄	
MAGNESIOCOULSONITE	MgV ₂ O ₄	
TEGENGRENITE	$(Mg,Mn^{2+})_2(Sb_{0.5}Mn^{3+}_{0.5})O_4$	
XIEITE	FeCr ₂ O ₄	(orth/Bbmm)
CHENMINGITE	FeCr ₂ O ₄	orth/Pnma
MAOHOKITE	MgFe ₂ O ₄	orth/Pnma`
GUITE	Co ²⁺ Co ³⁺ ₂ O ₄	cub/Fd3m
DELLAGIUSSTAITE	$V^{2+}AI_2O_4$	cub/Fd3m
THERMAEROGENITE	CuAl ₂ O ₄	cub/Fd3m
TSCHAUNERITE	(Fe ²⁺)(Fe ²⁺ Ti ⁴⁺)O ₄	orth/Cmcm
	NICHROMITE COCHROMITE ZINCOCHROMITE COULSONITE VUORELAINENITE ULVÖSPINEL QANDILITE MAGNESIOCOULSONITE TEGENGRENITE XIEITE CHENMINGITE MAOHOKITE GUITE DELLAGIUSSTAITE THERMAEROGENITE	NICHROMITE $(Ni,Co)(Cr,Fe)_2O_4$ COCHROMITE $(Co,Ni)(Cr,Al)_2O_4$ ZINCOCHROMITE $ZnCr_2O_4$ COULSONITE FeV_2O_4 VUORELAINENITE $(Mn,Fe)(V,Cr)_2O_4$ ULVÖSPINEL Fe_2TiO_4 QANDILITE $(Mg,Fe)_2(Ti,Fe,Al)O_4$ MAGNESIOCOULSONITE MgV_2O_4 TEGENGRENITE $(Mg,Mn^{2+})_2(Sb_{0.5}Mn^{3+}_{0.5})O_4$ XIEITE $FeCr_2O_4$ CHENMINGITE $FeCr_2O_4$ GUITE $Co^{2+}Co^{3+}_2O_4$ DELLAGIUSSTAITE $V^{2+}Al_2O_4$ THERMAEROGENITE $CuAl_2O_4$

SERIES P KORAGOITE, mon/P21. Structure consists of edge-sharing MnO6, NbO6 and TaO6 octahedra forming zigzag columns // [010] ; the columns are linked by W trigonal prisms.

DABPA KORAGOITE (Mn,Mn,Fe,•)₃(Nb,Mn)₂(Nb,Ta,W,•)₃(W,Ti,•)₂O₂₀

SERIES Q HAUSMANNITE, tetr/I4₁/amd. The structure is a distortion derivative of spinel. It is based on a cubic closest packing of oxygens, with Mn²⁺ in octahedral voids, and Mn⁴⁺ in tetrahedral voids.

DABQA	HAUSMANNITE	MnMn ₂ O ₄	
DABQB	HETAEROLITE	$ZnMn_2O_4$	
DABQC	HYDROHETAEROLITE	$Zn_2Mn_4O_8H_2O$	
DABQD	IWAKIITE	Mn(Fe,Mn) ₂ O ₄	(P4 ₂ /nnm)

SERIES R DEFECT FLUORITE Structure, tetr/l4₁/acd. The structure is based on a defect simple cubic packing of oxygen atoms with Mn atoms with two different co-ordinations, cubic and [6], and Si atoms with tetrahedral co-ordination. This structure can be considered as an interstitial substitution and defect derivative of fluorite.

DABRA	BRAUNITE	MnMn ₆ SiO ₁₂
DABRB	ABSWURMBACHITE	CuMn ₆ SiO ₁₂
DABRC	NELTNERITE	CaMn ₆ SiO ₁₂
DABRD	GAREDALITE	$ZrMn^{2+}{}_{2}Mn^{3+}{}_{4}SiO_{12}$

SERIES S SPINEL-Like structures, orth/lbmm. The structure of manganostibite includes populated octahedra edge-sharing chains...Mn-Mn-Sb-Mn-Mn-Sb... which run parallel to the y-axis and these further share edges with Mn-O octahedral edge-sharing walls. The walls are three octahedral wide along the y-axis and run parallel to the z-axis. The tetrahedra share corners with the octahedral and occur as [T₃O₁₀] triple groups. Manganostibite belongs to an homologous series, M_{2n}O_{n-1}[T_nO_{3n+1}], where n = 3; the simplest member of this series is the spinel structure type.

DABSA	MANGANOSTIBITE	Mn ₇ SbAsO ₁₂	
DABSB	KATOPTRITE	$Mn_{13}Sb_2AI_4Si_2O_{28}$	mon/C2/m
		0	

DABSC YEATMANITE

DABSD FILIPSTADITE

(Mn,Zn)₁₃Sb₂Si₄Zn₂O₂₈ tric/P1 (Mn,Mg)₂(Sb⁵⁺0.5Fe0.5)O₄

SERIES T DEFECT SPINEL STRUCTURES. The crystal structure of mayenite is described as an aluminate framework filed with disordered calcium and "extra" oxygen. The structure of harmunite consists of two symmetrically independent FeO₆ octahedra connected over common edges, forming double rutile-type $_{\circ}^{-1}$ [Fe₂O₆] chains. Four such double chains are further linked by common oxygen corners creating a tunnel-structure with large trigonal prismatic cavities occupied by Ca along [001]. The structure of shulamitite is intermediate between perovskite and brownmillerite. Wernerkrauseite is a CA-deficient structural analogue of harmunite. Sharyginite structure consists of double layers of corner-sharing (Tik Fe) O₆ octahedra, which are separated by single layers of (FeO₄ tetrahedra. Reference:

- Griffin, W.L., Gain, S.E.M., Bindi, L., Toledo, V., Cámara, F., Saunders, M., O'Reilly, S.Y. (2018): Carmeltazite, ZrAl2Ti4O11, a New Mineral Trapped in Corundum from Volcanic Rocks of Mt Carmel, Northern Israel. Minerals, 8, 601; <u>https://doi.org/10.3390/min8120601</u>

The new mineral species carmeltazite, ideally ZrAl2Ti4O11, was discovered in pockets of trapped melt interstitial to, or included in, corundum xenocrysts from the Cretaceous Mt Carmel volcanics of northern Israel, associated with corundum, tistarite, anorthite, osbornite, an unnamed REE (Rare Earth Element) phase, in a Ca-Mg-Al-Si-O glass. In reflected light, carmeltazite is weakly to moderately bireflectant and weakly pleochroic from dark brown to dark green. Internal reflections are absent. Under crossed polars, the mineral is anisotropic, without characteristic rotation tints. Reflectance values for the four COM wavelengths (Rmin, Rmax (%) (λ in nm)) are: 21.8, 22.9 (471.1); 21.0, 21.6 (548.3), 19.9, 20.7 (586.6); and 18.5, 19.8 (652.3). Electron microprobe analysis (average of eight spot analyses) gave, on the basis of 11 oxygen atoms per formula unit and assuming all Ti and Sc as trivalent, the chemical formula

(Ti3+3.60Al1.89Zr1.04Mg0.24Si0.13Sc0.06Ca0.05Y0.02Hf0.01)Σ=7.04O11. The simplified formula is ZrAl2Ti4O11, which requires ZrO2 24.03, Al2O3 19.88, and Ti2O3 56.09, totaling 100.00 wt %. The main diffraction lines, corresponding to multiple hkl indices, are (d in Å (relative visual intensity)): 5.04 (65), 4.09 (60), 2.961 (100), 2.885 (40), and 2.047 (60). The crystal structure study revealed carmeltazite to be orthorhombic, space group Pnma, with unit-cell parameters a = 14.0951 (9), b = 5.8123 (4), c = 10.0848 (7) Å, V = 826.2 (1) Å3, and Z = 4. The crystal structure was refined to a final R1 = 0.0216 for 1165 observed reflections with Fo > 4σ(Fo). Carmeltazite exhibits a structural arrangement similar to that observed in a defective spinel structure. The name carmeltazite derives from Mt Carmel ("CARMEL") and from the dominant metals present in the mineral, i.e., Titanium, Aluminum and Zirconium ("TAZ"). The mineral and its name have been approved by the IMA Commission on New Minerals, Nomenclature and Classification (2018-103).

DABTA	BROWNMILLERITE	Ca ₂ (Al,Fe)O ₅	orth/Ibm Perovskite deficient ty pe
DABTB	CHLORMAYENITE	Ca ₁₂ Al ₁₄ O ₃₃ Cl ₂	cub/l <u>4</u> 3d
DABTC	SREBRODOLSKITE	$Ca_2Fe_2O_5$	orth/Pnma deficient perovskite type
DABTD	GROSSITE	CaAl ₄ O ₇	mon/C2/c
DABTE	DMITRYIVANOVITE	CaAl ₂ O ₄	mon/P21/c
DABTF	BREARLEYITE	Ca ₁₂ Al ₁₄ O ₃₂ Cl ₂	cub/l <u>4</u> 3d
DABTG	SHULAMITITE	Ca ₃ TiFe ³⁺ AlO ₈	orth/Pmma deficient perovskite type
DABTH	DIAOYUDAOITE (?)	NaAl ₁₁ O ₁₇	hex/P6 ₃ /mmc
DABTI	HARMUNITE	CaFe ₂ O ₄	orth/Pnma
DABTJ	CHLORKYUYGENITE	Ca ₁₂ Al ₁₄ O ₃₂ [(H ₂ O) ₄ Cl ₂]	cub/l <u>4</u> 3d
DABTK	FLUORMAYENITE	Ca ₁₂ Al ₁₄ O ₃₂ F ₂	cub/l <u>4</u> 3d
DABTL	FLUORKYUYGENITE	Ca ₁₂ Al ₁₄ O ₃₂ [(H ₂ O) ₄ F ₂]	cub/l <u>4</u> 3d
DABTM	WERNERKRAUSEITE	Ca(Fe ³⁺ ,Mn ³⁺) ₂ Mn ⁴⁺ O ₆	orth/Pnma
DABTN	SHARYGINITE	Ca ₃ TiFe ₂ O ₈	orth/P2₁ma
DABTO	CARMELTAZITE	$ZrAI_2Ti_4O_{11}$	orth/Pnma
DABTP	KAHLENBERGITE	KAI ₁₁ O ₁₇	hex/P6 ₃ /mmc

SERIES U CALCIOTANTITE, hex/P6₃22. Structure consists of sheets of edge-sharing TaO₇ pentagonal dipyramids // [001] which are linked into a framework by TaO₆ octahedra and caO₈ polyhedra.

DABUA	CALCIOTANTITE	CaTa ₄ O ₁₁
DABUB	IRTYSHITE	Na ₂ (Ta,Nb) ₄ O ₁₁

DABUC NATROTANTITE NaTa₃O₈

SERIES V PETSCHECKITE, hex/P<u>3</u>1m. Structures not known. Mücke, A. & Strunz, H. (1978): Petscheckite and liandratite, two new pegmatite minerals from Madagascar. *American Mineralogist* 63: 941-946 - Tomašić, N., Raade, G. & Bermanec, V. (2004): REE-bearing petscheckite from Tiltvika, Nordland, Norway, and its heating products. *Neues Jahrbuch für Mineralogie Monatshefte* 2004 (4): 163-175

hex/P63 or P63/m

- DABVA PETSCHECKITE UFe(Nb,Ta)₂O₈
- DABVB LIANDRATITE U(Nb,Ta)₂O₈
- SERIES W SIMPSONITE, trig/P3. The structure is based on clusters of edge-sharing octahedra in close-packed layers along (001). The top layer contains the Ta octahedra while the lower layer contains the Al octahedra. The structure fits a HCP scheme.

DABWA SIMPSONITE Al₄(Ta,Nb)₃(O,OH,F)₁₄

- SERIES X SWEDENBORGITE, hex/P6₃mc. The structure is based on a <u>ch</u> closest packing of oxygens and Na atoms. The Sb atoms occupy 1/8 of the octahedral voids, and the Be atoms 1/4 of the tetrahedral voids. The structure is built by two alternate kind of layers.
- DABXA SWEDENBORGITE NaBe₄SbO₇
- SERIES Y CALZIRTITE SERIES-CaF₂-CeO₂ Structure, CN = 7, tetr/l4₁/acd. Structure consists of a distorted fluorite-type structure consisting of a framework of edge- and corner-sharing ZrO_{7-8} polyhedra and CaO₆ and TiO₆ octahedra.

DABYACALZIRTITECaZr3TiO9DABYBHIÄRNEITECa2(Zr,Ti)5(Sb,Mn)2O16

- DABYC TAZHERANITE (Zr,Ca,Ti)O₂
- SERIES Z LÅNGBANITE, trig/P31m. The structure of this complex mineral is based on "double hexagonal" close packing of cations in the sequence ABAC. Unlike the cations, the anion arrangement is not based on principles of close packing. The structure is conceived as consisting of four discrete layers which link by corner and edge sharing. At z=0, the ${}^2_{-1}$ [Mn9²⁺Sb3⁵⁺O24] ordered brucite-like sheet has a [M3O8] unit that mimics the octahedral sheet of spinel along [111]. At z = 1/4, the [Mn9³⁺O6(SiO4)(SiO4)2O18] unit relates to a sheet in schairerite and to the fundamental sheet in mitridatite. At z = 1/2, the [Mn3²⁺O6Mn9³⁺O23] sheet relates to pyrochlore and the large alunite-jarosite family. At z = 3/4, the [Mn9³⁺O3(SiO4)3O18O3] sheet is based on Mn3OO12 islands of three Mn-O atom distorted octahedra comprising three shared edges and one shared vertex, all nearly in a plane. Langbanite is considered to be an oxide-stuffed version of the La inter-metallic structure.

DABZA LÅNGBANITE Mn₄Mn₉SbSi₂O₂₄

SERIES 27 FEIITE, orth/Cmcm.

DAB27A FEIITE $Fe^{2+}Z(Fe^{2+}Ti^{4+})O_5$

GROUP B FRAMEWORK STRUCTURES

TYPE A SIMPLE

SERIES A ANATASE, tetr/l4₁/amd. The structure is based on the cubic closest packing of oxygen atoms, where the Ti atoms are located in octahedral voids. On the layer parallel to (001) the Ti atoms show a square pattern, but in the plane parallel to the closest packed layers, the Ti atoms show a zig-zag pattern.

DBAAA ANATASE

- SERIES B ICE, hex/P6₃/mmc. The structure is similar to that of tridymite but the relative size of the atoms forming the tetrahedra is inverted; instead of SiO₄ tetrahedra, it is based on O^tH₄ tetrahedra. In the ice structure, each H₂O molecule is tetrahedrally coordinated to four neighboring H₂O molecules, analogous to Si in beta-tridymite.
- DBABA ICE H₂O

SERIES C KROTITE, mon/P2₁/n. The structure is a stuffed derivative of tridymite.

- DBACA KROTITE CaAl₂O₄ mon/P2₁/n
- TYPE B COMPLEX

SERIES A PEROVSKITE SERIES, orth/Pnma. The structure is based on a cubic closest packing of oxygen and calcium atoms with Ti atoms occupying 1/4 of the octahedral voids with a square pattern. Structure consists of M octahedra share corners to create a 3-dimensional framework with cavities that accommodate the M cations.

On the basis of extensive studies of synthetic perovskite-structured compounds it is possible to derive a hierarchy of hettotype structures which are derivatives of the arisotypic cubic perovskite structure (ABX3), exemplified by SrTiO3 (tausonite) or KMgF3 (parascandolaite) by: (1) tilting and distortion of the BX6 octahedra; (2) ordering of A- and B-site cations; (3) formation of A-, B- or X site vacancies. This hierarchical scheme can be applied to some naturally-occurring oxides, fluorides, hydroxides, chlorides, arsenides, intermetallic compounds and silicates which adopt such derivative crystal structures. Application of this hierarchical scheme to naturally-occurring minerals results in the recognition of a perovskite supergroup which is divided into stoichiometric and non stoichiometric perovskite groups, with both groups further divided into single ABX3 or double A2BBX6 perovskites, Subgroups, and potential subgroups, of stoichiometric perovskites include: (1) silicate single perovskites of the bridgmanite subgroup; (2) oxide single perovskites of the perovskite subgroup (tausonite, perovskite, loparite, lueshite, isolueshite, lakargiite, megawite); (3) oxide single perovskites of the macedonite subgroup which exhibit second order Jahn-Teller distortions (macedonite, barioperovskite); (4) fluoride single perovskites of the neighborite subgroup (neighborite, parascandolaite); (5) chloride single perovskites of the chlorocalcite subgroup (6) Bsite cation ordered double fluoride perovskites of the cryolite subgroup (cryolite, elpasolite; simmonsite); (7) B-site cation ordered oxide double perovskites of the vapnikite subgroup (vapnikite, (?) latrappite). Non-stoichiometric perovskites include: (1) A-site vacant double hydroxides, or hydroxide perovskites, belonging to the söhngeite, schoenfliesite, and stottite subgroups; (2) Aniondeficient perovskites of the brownmillerite subgroup (srebrodolskite, shulamitite); (3) A-site vacant quadruple perovskites (skutterudite subgroup); (4) B-site vacant single perovskites of the oskarssonite subgroup [oskarssonite,waimirite-(Y)]; (5) B-site vacant inverse single perovskites of the cohenite and auricupride subgroups; (6) B-site vacant double perovskites of the diaboleite subgroup; (7) anion-deficient partly-inverse B-site quadruple perovskites of the hematophanite subaroup.

DBBAA	PEROVSKITE	CaTiO ₃	
DBBAB	LATRAPPITE	(Ca,Na)(Nb,Ti)O ₃	
DBBAC	LOPARITE-(Ce)	(Ce,Na,Ca)(Ti,Nb)O ₃	
DBBAD	LUESHITE	NaNbO ₃	
DBBAE	TAUSONITE	SrTiO₃	
DBBAF	MACEDONITE	PbTiO ₃	tetr/P4/mmm
DBBAG	NATRONIOBITE ?	NaNbO₃	mon/
DBBAH	ISOLUESHITE	(Na,Ca,La)(Nb,Ti)O ₃	Pm3m
DBBAI	BARIOPEROVSKITE	BaTiO₃	Orth/Amm2
DBBAJ	LAKARGIITE	CaZrO ₃	OrthPnma
DBBAK	MEGAWITE	CaSnO₃	orth/Pbnm
DBBAL	NATALIAKULIKITE	Ca ₄ Ti ₂ (Fe ³⁺ Fe ²⁺)(Si,Fe ³⁺ ,A	l)O ₁₁ orth/Pnma
DBBAM	VAPNIKITE	Ca ₃ UO ₆	mon/P2 ₁ /n
DBBAN	PARASCANDOLAITE	KMgF₃	iso/Pm3
WAAA29	BRIDGMANITE	MgSiO ₃	orth/Pnma
		40	

DBBAO GOLDSCHMIDTITE

KNbO₃

iso/Pm3m

SERIES B AESCHYNITE SERIES, orth/Pbnm. The structure consists of double chains of B octahedra linked in pairs by sharing edges, and extending indefinitely along b by sharing corners. The large A cations are accommodated in 8-coordinated sites in channels between the chains of octahedra, and the size of the site can be adjusted by rotating the octahedral chains about their common corners. Structure consists of dimmers of edge-sharing (Nb,Ta,Ti)O₆ octahedra sharing corners to form zigzag chains // [010]; REE polyhedra share edges to form chains // [010]; each REE polyhedron shares edges with six (Nb,Ta,Ti) octahedra to form a framework.

DBBBA	AESCHYNITE-(Ce)	(Ce,Ca,Fe,Th)(Ti,Nb) ₂ (O,OH) ₆
DBBBB	AESCHYNITE-(Nd)	(Nd,Ce,Ca)(Ti,Nb) ₂ (O,OH) ₆
DBBBC	AESCHYNITE-(Y)	(Y,Ca,Fe,Th)(Ti,Nb) ₂ (O,OH) ₆
DBBBD	NIOBO-AESCHYNITE-(Ce)	(Ce,Ca,Th)(Nb,Ti) ₂ (O,OH) ₆
DBBBE	NIOBO-AESCHYNITE-(Nd)	(Nd,Ce)(Nb,Ti) ₂ (O,OH) ₆
DBBBF	TANTALAESCHYNITE-(Y)	(Y,Ce,Ca)(Ta,Ti,Nb) ₂ O ₆
DBBBG	RYNERSONITE	Ca(Ta,Nb) ₂ O ₆
DBBBH	VIGEZZITE	(Ca,Ce)(Nb,Ta,Ti) ₂ O ₆
DBBBI	NIOBOAESCHYNITE-(Y)	[(Y,Ln)Ca,Th,Fe](Nb,Ti,Ta) ₂ (O,OH) ₆
DBBBJ	LORANSKITE-(Y)	(Y,Ce,Ca)ZrTaO ₆
DBBBK	KOBEITE-(Y)	(Y,U)(Ti,Nb) ₂ (O,OH) ₆

- SERIES C TANTITE, tric/P1. Structure not known. Mineralogicheskii Zhurnal, Kiev (1983): 5(3): 90-93.American Mineralogist (1984): 69: 1193.
- DBBCA TANTITE (Ta,Nb)₂O₅
- WELINITE, hex/P3. Structure consists of edge- and corner-sharing Mn²⁺ octahedra forming a SERIES D framework with insular Si tetrahedra; channels // {0001] contain partially occupied chains of facesharing V⁵⁺ octahedra. The new mineral barwoodite (IMA2017-046), Mn2+6(Nb5+,□)2(SiO4)2(O,OH)6, was found in miarolitic cavities at the Big Rock guarry (also known as the 3M guarry), Granite Mountain, Little Rock, Pulaski County, Arkansas, USA. It is interpreted as crystallizing from peqmatitic fluids. The mineral occurs as brownish-red hexagonal plates up to 3 mm in diameter. Crystals are transparent with vitreous luster and light orange streak. The tenacity is brittle, the Mohs hardness is approximately 3¹/₂, the fracture is curved, and there is one perfect cleavage on {001}. The calculated density for the empirical formula is 4.227 g/cm³. Barwoodite is optically uniaxial (–) with ω = 1.873(3) and ε = 1.855(5) (white light) and is nonpleochroic. Electron microprobe analyses (WDS mode) provided the empirical formula Mn2+6(Nb5+0.94Fe3+0.18Mn3+0.11□0.77)Σ2(SiO4)2[O3.58(OH)2.42]Σ6. The six strongest X-ray powder diffraction lines are [dobs Å(I)(hkl)]: 3.125(95)(11-1), 2.858(56)(021), 2.688(57)(210), 2.349(81)(300), 1.7930(100)(212), and 1.5505(75)(140,-3-21). Barwoodite is trigonal, P3, a 8.2139(10), c 4.8117(4) Å, V 281.14(7) Å3, and Z = 1. The structure determination for barwoodite (R1 = 0.0246 for 746 reflections with $lo > 2\sigma l$) shows it to be isostructural with welinite, franciscanite, and örebroite. Together, these four minerals comprise the welinite group.

DBBDA	ÖREBROITE	Mn ₆ (Sb,Fe) ₂ Si ₂ (O,OH) ₁₄
DBBDB	FRANCISCANITE	Mn ₆ (V,□) ₂ Si ₂ (O,OH) ₁₄
DBBDC	WELINITE	$Mn_6(W,Mg)_2Si_2(O,OH)_{14}$
DBBDD	BARWOODITE	$Mn^{2+}{}_{6}Nb^{5+}(SiO_{4})_{2}O_{3}(OH)_{3}$
DBBDE	SCORTICOITE	$Mn_6(Sb\square)_2(SiO_4)_2O_3(OH)_3$

SERIES E EYSELITE, orth/P. Structure not known due to small size of crystals. Roberts, A.C., Seward, T.M., Reusser, E., Carpenter, G.J.C., Grice, J.D., Clark, S.M., and Marcus. M.A. (2004): Eyselite, Fe3+Ge4+307(OH), a new mineral species from Tsumeb, Namibia. Canadian Mineralogist, 42, 1771-1776.

DBBEA EYSELITE

Fe³⁺Ge⁴⁺₃O₇(OH)

DBBEB	CESPLUMTANITE 501.	$Cs_2Pb_3Ta_8O_{24}$	tetr. n/s known American Mineralogist (1989): 74:
	0011		

SERIES F DERBYLITE, mon/P2₁/m. The structure is based on a closest-packed anion framework with a stacking sequence (hhc...). Small cations are ordered into 14 of the 30 octahedral sites per unit cell, forming α -PbO₂ and V₃O₅-type chains of edge-shared octahedra along [001]. In the cubic stacked anion layers, two anions per unit cell, are missing, forming cubo-octahedral cavities that are occupied by Ba, and by As³⁺₂ pairs. The structure of batisivite is a combination of zigzag double chains of octahedra of α -PbO₂-type and columns of V₂O₅-type. The channels formed by these structural units can be described as chains of cuboctahedral cavities running // to [011]. Ti, V, Cr, Fe, and Nb occupy the octahedral sites, whereas Ba and Si-O groups occupy the cuboctahedral sites.

DBBFA	DERBYLITE	Fe ₄ Ti ₃ SbO ₁₃ (OH)
DBBFB	TOMICHITE	(V,Fe) ₄ Ti ₃ AsO ₁₃ (OH)
DBBFC	HEMLOITE	(As,Sb) ₂ (Ti,V,Fe,Al) ₁₂ O ₂₃ (OH)
DBBFD	GRAESERITE	(Fe,Ti) ₄ Ti ₃ AsO ₁₃ (OH)
DBBFE	BATISIVITE	V ₈ Ti ₆ [Ba(Si ₂ O ₇)]O ₂₂

SERIES G PEROVSKITE DERIVATIVE Structures. The structure is based on the stacking of four perovskite-like cells along [001].

DBBGA	HEMATOPHANITE	Pb ₄ Fe ₃ O ₈ Cl	tetr/P4mm

MENEZESITE, cubic/Im3. The main building unit of the structure is the $[MgW_{12}O_{42}]^{10}$ SERIES H heteropolyanion, formed by 12 face and corner sharing WO6-octahedra, enclosing a 12-fold coordinated cavity, which is occupied by Mg. The heteropolyanions occupy the corners and the body centered positions of the unit cell and are cross-linked in 3D by MgO6-octahedra to form a rigid 3D lattice in two ways. In the first, Mg (1) links the central polyanions to its eight neighbors in the corners of the unit cell, whereas, in the second, Mg (2) links the polyanions with their six neighbors across the unit-cell faces. These latter cations complete their octahedral coordinations with equatorial OH anions and water molecules in relation 1:2 to reach the electroneutrality of the compound. Am. Min. 93, 81.

DBBHA	MENEZESITE	Ba ₂ MgZr ₄ (BaNb ₁₂ O ₄₂).12H ₂ O
DBBHB	ASPEDAMITE	$\square_{12}(Fe^{3+}{}_2Fe^{2+})Nb_4(ThNb_9Fe^{3+}{}_2Ti^{4+}O_{42})((H_2O)_9(OH)_3$

BILLWISEITE, mon/C2/c. The structure consists of two distinct sheets of (Ta,Nb,W) octahedral and SERIES I three distinct sheets of Sb³⁺ polyhedra // to (100). These sheets alternate in the a direction to form a continuous structure.

Sb³⁺5Nb₃WO₁₈ DBBIA BILLWISEITE

RANKAMAITE, orth/Cmmm. In the rankamaite structure, the Ta atoms are coordinated by six and SERIES J seven oxygen atoms in the form of distorted TaO_6 octahedra and TaO_7 pentagonal bipyramids. respectively. Every pentagonal bypramid shares edges with four octahedral, thus forming Ta₅O₁₄ units. The K atom is in an 11-fold coordination, whereas one Na atom is in a 10-fold and the other is in a 12-fold coordination.

DBBJA	RANKAMAITE	$(Na_{2.21}K_{1.26})_{3.37}(Ta_{9.12}Nb_{1.30}AI_{0.59})_{11}[O_{26.3}(OH)_{4.7}]_{31}$
DBBJB	SOSEDKOITE	(K,Na) ₅ Al ₂ (Ta,Nb,Sb) ₂₂ O ₆₀

SERIES K TASHELGITE, mon/Pc. Rastsvetaeva, R.K., Aksenov, S.M., Verin, I.A. (2010): Crystal structure of complex natural aluminum magnesium calcium iron oxide. Crystallography Reports, 55, 563-568.

> Rastsvetaeva, R.K., Aksenov, S.M., Chukanov, N.V. (2010): Structure of the tashelgite mineral Ca2Mg2Fe22+Al18O32(OH)2 from Western Siberia: A new structure type. Doklady Chemistry, 434, 233-236.

Ananyev, S.A. et al (2010), Tashelgite, IMA 2010-017. CNMNC Newsletter, August 2010, p.798, *Mineralogical Magazine* 74, 797-800.

Ananyev, S.A., Konovalenko, S.I., Rastsvetaeva, R.K., Aksenov, S.M., Chukanov, N.V., Sapozhnikov, A.N., Zagorsky, V.E. & Virus, A.A. (2011): Tashelgite, CaMgFe2+Al9O16(OH), a new mineral species from calc-skarnoid in Gorny Shoria. *Zapiski Rossiyskogo Mineralogicheskogo Obshchestva*, **140(1)**, 49-57 (in Russian). English translation: *Geology of Ore Deposits*, **53**, 751-757.

- DBBKA TASHELGITE CaMgFe³⁺Al₉O₁₆(OH)
- SERIES L ROSIAITE, trig/P<u>3</u>1m. Structure consists of gibbsite-like layers of edge-sharing SbO₆ octahedra // (0001), with 1/3 of the octahedral sites vacant, and are linked by PbO₆ octahedra situated above and below the vacant sites of the Sb layers.
- DBBLA ROSIAITE PbSb₂O₆
- SERIES M LUCASITE, mon/l2/a. The structure is related to the PbSb₂O₆-type structure, with ordering of Ce and Ti atoms in alternate {001} cations layers in a hexagonal closest-packed anion arrangement. The Ticentered octahedra share edges to form gibbsite-like fused hexagonal rings. The Ce atoms are sandwiched between pairs of hexagonal rings and are displaced by 0.5 A along [010] from the centers of octahedral sites to adopt eightfold co-ordination.
- DBBMA LUCASITE-(Ce) (Ce,La)Ti₂(O,OH)₆
- DBBMB KASSITE Ca[Ti₂O₄(OH)₂]
- SERIES N CAFETITE, mon/P2₁/n. The TiO₆ octahedra form [Ti₂O₅] sheets parallel to (001). The Ca atoms and water groups are located between the sheets to form a three-dimensional structure.
- DBBNA CAFETITE Ca[Ti₂O₅](H₂O)
- SERIES O BACKITE, trig/P312. Tait, K.T., DiCecco, V., Cooper, M.A., Ball, N.A. and Hawthorne. F.C. (2014) Backite, IMA 2013-113. CNMNC Newsletter No. 19, February 2014, page 169; Mineralogical Magazine, 78, 165-170.

Tait, K.T., DiCecco, V., Ball, N.A., Hawthorne, F.C., Kampf, A.R. (2014): Backite, Pb2Al(TeO6)Cl, a new tellurate mineral from the Grand Central Mine, Tombstone Hills, Cochise County, Arizona: Description and crystal structure. *Canadian Mineralogist*, **52**, 935-942

- DBBOA BACKITE Pb₂AITeO₆CI MOVE TO TELLURATES
- SERIES P TEWITE, orth/Pban. Tewite, with end-member formula (K1.5□0.5)Σ2(Te4+1.25W0.25□0.5)Σ2W5O19 or K1.5(Te1.25W0.25)Σ1.5W5O19, is a new mineral species (IMA2014-053), discovered in the vicinity of Nanyang village, Huaping County, located in the south of the Panzhihua-Xichang region, southwestern China. Tewite occurs in the Neoproterozoic Sinian light-weathered biotite-quartz monzonite, near the contact zone with gabbro. The associated minerals are alkali feldspar, biotite, clinoamphibole, ilmenite, zircon, zoisite, tourmaline, monazite-(Ce), allanite-(Ce), scheelite, tellurite and the new mineral wumuite (KAI0.33W2.67O9, IMA2017-067a), in addition to an unidentified, potentially new mineral corresponding to WO3. Tewite forms platy crystals that range from 0.08 × 0.1 × 0.1 to 0.1 × 0.2 × 0.5 mm in size. The crystals are greenish yellow, with a light-yellow to white streak, translucent to transparent, and with adamantine luster. Mohs hardness is $3\frac{1}{2}-4$, and the tenacity is brittle. It has perfect {100}, {001}, and {010} cleavages, and the calculated density is 6.903 q/cm3. The mineral is biaxial positive with $2V = 70^{\circ}$. The Gladstone–Dale relationship predicts an average index of refraction of 2.04. The chemical composition determined by wavelength-dispersive electron-microprobe analysis is (wt%, average of n = 16): Na2O 0.13, K2O 5.08, WO3 83.34, TeO2 11.32, total 99.86. The empirical formula, based on 19 O, is (K1.61Na0.06□0.33)Σ2.00(Te1.06W0.35□0.59)Σ2.00W5O19. The eight strongest X-ray powderdiffraction lines [d in Å (l) (hkl)] are: 6.486 (50) (040), 3.8333 (100) (001), 3.6212 (30) (200), 3.1983 (65) (080), 2.4541 (50) (081), 1.8442 (30) (390), 1.6365 (25) (401), and 1.5743 (55) (480). Refinement of the crystal structure (R1 = 0.075) gave the following data: orthorhombic, space group Pban, a = 7.2585(4), b = 25.8099(15), c = 3.8177(2)Å, Z = 2. Tewite has a new tungsten-bronze (TB)-type derivative structure. Distorted TeO6 octahedra break TB slabs into ribbons which are displaced by ½

a relative to their neighbors, while K partly occupies two mutually exclusive sites in hexagonal

channels || c. Short-range order and displacement of K ions are likely responsible for an observed incommensurate modulation of the average structure indicated by week satellite reflections, which were not considered in the structure refinement. The formation of the mineral may be related to the nearby quartz-vein-type Au mineralization; the mineral is formed by the metasomatic reaction of a high-temperature fluid rich in W and Te with the potassium feldspar in the monzonite. Tewite is a mineralogically unique K–Te–W oxide. The mineral is classified as a composite oxide, New Dana Classification class 07.04.03, of stoichiometry A2B2C5O19.

http://www.cugb.edu.cn/uploadCms/outCampusHtml/2014/40100/20140917173131168166.shtml

Li, G., Xue, Y. and Xiong, M.(2014) Tewite, IMA 2014-053. CNMNC Newsletter No. 22, October 2014, page 1245; *Mineralogical Magazine*, 78, 1241-1248.

DBBPA TEWITE K2(Te1.5X0.5)2W5O19

SERIES Q TULULITE, cub/F23. The tetrahedral framework of tululite is formed by T₇O₁₃ secondary building blocks, which consist of four corner-linked tetrahedra sharing a common oxygen atom and three tetrahedra sharing two O atoms with the neighbor SBU. Ca cations occupy three positions; two of them also contain a minor amount of Cd. The Ca sites surround an island (Fe, AI)O₆ octahedron and a (Si,P)O₄ tetrahedron in the centers of framework cages at the junction of eight SBUs. The (Fe,AI)O₆ octahedron is coordinated by 14 Ca positions into a 6-capped cube, whereas the (Si,P)O₄ tetrahedron is coordinated by six Ca positions into a regular octahedron. Khoury, H.N., Sokol, E.V., Kokh, S.N., Seryotkin, Y.V., Nigmatulina, E.N., Goryainov, S.V., Belogub, E.V. and Clark, I.D. (2015) Tululite, IMA 2014-065. CNMNC Newsletter No. 23, February 2015, page 53; *Mineralogical Magazine*, **79**, 51-58.

- DBBQA TULULITE Ca₁₄(Fe,Al)(Al,Zn,Fe,Si,P,Mn,Mg)₁₅O₃₆
- SERIES R LANGHOFITE, tric/P1

DBBRA LANGHOFITE Pb₂(OH)[WO₄(OH)]

- GROUP C RING STUCTURES
- GROUP D INSULAR STRUCTURES
- TYPE A SIMPLE
- SERIES A ARSENOLITE SERIES, cub/Fd3m. The structure consists of As₂O₆ molecules packed together in the unit cube in the same manner as are the carbon atoms in the diamond structure. Within the molecule, each As (Sb) atom has three oxygen neighbors at a distance that is 1.80 A. Structure consists of four flat trigonal pyramids of MO₃ forming O-sharing M₄O₆ molecules that are linked by van der Waals bonding.
- DDAAA ARSENOLITE As₂O₃
- DDAAB SENARMONTITE Sb₂O₃

GROUP E CHAIN STRUCTURES

TYPE A SIMPLE

SERIES A RUTILE SERIES, tetr/P4₂/mnm. Structure consists of edge-sharing M octahedra form straight chains // [001]; the chains are linked by sharing corners of the octahedra.

DEAAA	RUTILE	TiO ₂
DEAAB	PYROLUSITE	MnO_2
DEAAC	CASSITERITE	SnO_2
DEAAD	PLATTNERITE	PbO ₂
DEAAE	ARGUTITE	GeO ₂
DEAAF	STISHOVITE	SiO ₂
DEAAG	TRIPUHYITE	${\sf FeSbO}_4$
DEAAH	open	

DEAAI open

DEAAJ VARLAMOFFITE

Sn_{1-x}Fe_xO_{2-x}(OH)_x

SERIES B Open

SERIES C RAMSDELLITE, orth/Pbnm. The structure is based on a hexagonal closest packing of oxygens, with one half of the octahedral voids occupied by Mn atoms, forming a double row pattern. The double rows on the adjacent layers are placed over the empty rows, that is in between the double rows of the adjacent layers. Structure consists of edge-sharing M octahedra forming double chains // [001], as in diaspore; the chains are linked by sharing corners of octahedra, creating channels // [001] that may contain small cations.

DEACA	RAMSDELLITE	MnO ₂	
DEACB	PARAMONTROSEITE	VO ₂	
DEACC	NSUTITE	γ MnO 2	hex/P6 ₃ /mmc
DEACD	AKHTEMSKITE	εMnO2	

- SERIES D DOWNEYITE, tetr/P4₂/mbc. The structure consists of endless strings in which half of the oxygen atoms join the Se atoms and the other oxygens are bound only to one Se. The SeO₂ strings extending parallel to one another and to the c_o axis can be imagined as flat SeO₃ pyramids that have selenium atoms at the apexes and oxygen atoms linking them to one another. These pyramids are nearly regular. Structure consists of corner-sharing SeO₃ pyramids forming isolated chains // [001]; the chains are linked by electrostatic interactions.
- DEADA DOWNEYITE SeO₂
- SERIES E VALENTINITE, orth/Pccn. Structure consists of corner-sharing SbO₃ trigonal pyramids forming chains // [001].
- DEAEA VALENTINITE Sb₂O₃
- SERIES F MONTROYDITE, orth/Pnma. Structure consists of infinite zigzag chains of Hg-O-Hg atoms running // [100]; the chains are packed into layers // (010).
- DEAFA MONTROYDITE HgO
- SERIES G KYZYLKUMITE-SCHREYERITE SERIES, mon/P2₁/c. The structures can be derived from that of alpha PbO₂ by crystallographic shear // (110). Byrudite has the norbergite-type structure. The structure is based on a hexagonal closest packing of O, OH and F, with Mg atoms in octahedral voids forming a zigzag pattern, and Si atoms in tetrahedral voids. The serrated chain of edge-sharing octahedra consists of five unique octahedra. It can be imagined derived from olivine and brucite. The structure of Kyzylkumite has a modular structure based on hexagonal close packing of O atoms, which are made up of rutile and montroseite slices. In tivanite the rutile:montroseite ratio is 1:1, in kyzylkumite the ratio is 2:1. The common structure type of oxyvanite and berdesinskiite can be described by hexagonal closest O packing with 3/5 of the octahedral voids occupied. Site-occupancy refinements support previous studies on synthetic V₂TiO₅ and V₃O₅ indicating that a strongly distorted octahedrally coordinated site, forming pairs of face-sharing octahedral.

DEAGA	KYZYLKUMITE	$Ti_2V^{3+}O_5(OH)$	mon/P21/c
DEAGB	SCHREYERITE	V ₂ Ti ₃ O ₉	C2/c
DEAGC	OLKHONSKITE	(Cr,V) ₂ Ti ₃ O ₉	C2/c,Cc,P2 ₁ /c,P2/c,Pc
DEAGD	BERDESINSKIITE	V ₂ TiO ₅	C2/c or Cc
DEAGE	OXYVANITE	V ₃ O ₅	C2/c
DEAGF	BYRUDITE	(Be,□)(V ³⁺ ,Ti) ₃ O ₆	orth/Pnma
DEAGG	TIVANITE	(TiO ₂)(VO(OH))	P2 ₁ /c

DEAGH	KLEBERITE	FeTi ₆ O ₁₁ (OH) ₅	mon/P21/c
DEAGI	VERBIERITE	BeCr ³⁺ ₂ TiO ₆	
DEAGJ	MACHIITE	Al ₂ Ti ₃ O ₉	mon/C2/c
DEAGK	VESTAITE	(Ti ⁴⁺ Fe ²⁺)Ti ⁴⁺ ₃ O ₉	mon/C2/c
DEAGL	DAITIANITE	Ti ³⁺ ₂ Ti ⁴⁺ O ₅	mon/C2/c

SERIES H CARMICHAELITE, mon/P2₁/c. The structure consists of stacked chains of cation octahedra in an `array of hexagonal closed-packed oxygen atoms, the hcp layers being parallel to (010).

DEAHA CARMICHAELITE

(Ti,Cr,Fe,Mg,Al)O_{1.5}(OH)_{0.5}

- SERIES I BIEHLITE, mon/2C/c. Structure consists of edge-sharing MoO₆ octahedra forming zigzag chains // (001) that are flanked on two sides by Sb₂O₂ groups; the resulting ribbons are linked by weak Sb-O bonds.
- DEAIA BIEHLITE (Sb,As)²MoO₆
- TYPE B COMPLEX
- SERIES A RUTILE DERIVATIVE Structure, tetr/P4₂/mnm. The structure of this series is based on a hexagonal closest packing with the Ta and Fe atoms occupying one half of the octahedral voids, with a row pattern. The structure is a substitution derivative of the rutile structure and is identical to the Sb^o₂Zn^o[O₆]^h inorganic structure type. The prominent feature of the structure is the presence of distorted, edge-sharing octahedra that form straight chains parallel to [001]. These chains have an intra-chain stacking sequence, ...A-B-B-A-B-B..., where A represents Fe²⁺ and B represents Ta in the ideal structural formula. Adjacent chains are linked by shared corners of the octahedra.

DEBAA	BYSTRÖMITE	MgSb ₂ O ₆
DEBAB	TAPIOLITE-(Fe)	(Fe,Mn)(Ta,Nb) ₂ O ₆
DEBAC	TAPIOLITE-(Mn)	(Mn,Fe)(Ta,Nb) ₂ O ₆
DEBAD	ORDONEZITE	$ZnSb_2O_6$
DEBAE	TREDOUXITE	NiSb ₂ O ₆

SERIES B ALPHA PbO₂ Substitution Derivative Structure, mon/P2/c. The structure is based a hexagonal closest packing where the Fe and W atoms are located in one half of the octahedral voids, the Fe and the W atoms form a zigzag pattern like in brookite. The layers parallel to (100) containing the Fe atoms alternate with the layers containing the W atoms. The structure is a distortion derivative of ixiolite, and a substitution derivative of alpha PbO₂.

DEBBA	SANMARTINITE	ZnWO ₄
DEBBB	HEFTETJERNITE	ScTaO ₄
DEBBC	FERBERITE	FeWO ₄
DEBBD	HÜBERNITE	MnWO ₄
DEBBE	HUANZALAITE	MgWO ₄
DEBBF	ROSSOVSKYITE	(Fe ³⁺ ,Ta)(Nb,Ti)O ₄

SERIES C ALPHA PbO₂ Derivative Structure, orth/Pcan, mon/C2/c. The structure is composed of coordination polyhedra which link via edge-sharing to form alpha PbO-like zigzag chains along z. Chains are interconnected by corner-sharing linkages between levels of the closest-packed layering. The A and B polyhedra alternate along the zigzag chains of their level; adjacent levels necessarily consist only of chains of C polyhedra. The structure of lithiotantite is composed of a slightly distorted hexagonal close-packed array of O atoms stacked in the [-101] direction, with the metal atoms occupying half of the octahedral sites. Thee are four symmetrically non-equivalent cations sites, with three of them occupied mainly by (Ta⁵⁺ + Nb⁵⁺) and one by Li⁺. The four distinct octahedral share edges, forming two types of zigzag chains (A and B) extending along the b axis. The A chains are built exclusively

of (Ta,Nb)O₆ octahedra (M1 and M2), whereas the B chains consist of alternating (Ta, Nb)O₆ and LiO₆ octahedra (M3 and M4, respectively).

DEBCA	IXIOLITE	(Ta,Fe,Sn,Nb,Mn)₄O ₈	
DEBCB	ACHALAITE	(Fe,Mn)(Ti,Fe,Ta)(Nb,Ta) ₂ O ₈	
DEBCC	WODGINITE	(Ta,Nb,Sn,Mn,Fe) ₁₆ O ₃₂	
DEBCD	SAMARSKITE-(Y)	YFe ³⁺ Nb ₂ O ₈	(mon, C2/c)
DEBCE	LITHIOWODGINITE	(Li,Mn,Fe)(Ta,Nb,Sn) ₃ O ₃₂	
DEBCF	FERROWODGINITE	FeSnTa ₂ O ₈	
DEBCG	TITANOWODGINITE	MnTiTa₂O ₈	
DEBCH	SAMARSKITE-(Yb)	[(Yb + Y),U,Th,Ca,Fe](Nb,Ta,Ti)O ₄	
DEBCI	FERROTITANOWODGINITE	FeTi(Ta,Nb) ₂ O ₈	
DEBCJ	LITHIOTANTITE	Li(Ta,Nb) ₃ O ₈	
DEBCK	SRILANKITE	Ti(Ti,Zr)O ₄	
DEBCL	CALCIOSAMARSKITE	(Ca,Fe,Y)(Nb,Ta) ₂ O ₈	
DEBCM	TANTOLOWODGINITE	(Mn, □)TaTa₂O ₈	
DEBCN	EKEBERGITE	ThFeNb ₂ O ₈	

SERIES D COLUMBITE, orth/Pcan. The structure is based on a hexagonal closest packing, with the Fe and Nb atoms located in half of the octahedral voids, forming a zigzag pattern, similar to the arrangement in anatase and brookite. The layers containing the iron atoms alternate with pairs of layers containing the Nb atoms in rows of zigzag edge-sharing octahedra. This structure is a substitution derivative of wolframite, or still of α - Pb^o[O₂]^h.

DEBDA	COLUMBITE-(Mn)	(Mn,Fe)(Nb,Ta) ₂ O ₆
DEBDB	TANTALITE-(Mn)	(Mn,Fe)(Ta,Nb) ₂ O ₆
DEBDC	COLUMBITE-(Fe)	(Fe,Mn)(Nb,Ta) ₂ O ₆
DEBDD	TANTALITE-(Fe)	FeTa ₂ O ₆
DEBDE	COLUMBITE-(Mn)	(Mg,Fe,Mn)(Nb,Ta) ₂ O ₆
DEBDF	TANTALITE-(Mg)	(Mg,Fe)(Ta,Nb) ₂ O ₆
DEBDG	QITIANLINGITE	(Fe,Mn) ₂ (Nb,Ta) ₂ WO ₁₀

SERIES E THOREAULITE, mon/C2/c. The structure consists of alternations of two types of layers perpendicular to x. One type of layer consists of corner-linked NbO₆ octahedra forming a flat, perforated, two-octahedron-thick sheet with closest-packed anions. The other type consists of distorted, edge-sharing Sn²⁺O₈ square antiprisms forming a flat, perforated sheet. The Sn²⁺ coordination polyhedron is severely distorted owing to the presence of a stereoactive lone-pair of electrons.

DEBEA	THOREAULITE	SnTa ₂ O ₆
DEBEB	FOORDITE	Sn(Nb,Ta) ₂ O ₆

- SERIES F PSEUDOBROOKITE SERIES, orth/ Pbmm. Structure consists of edge- and corner-sharing MO₆ octahedra forming bands // [010]; the bands share edges with adjacent bands, creating channels // [010].
- DEBFAPSEUDOBROOKITE Fe_2TiO_5 DEBFBARMALCOLITEMgTiTiO_5
- SERIES G CRYPTOMELANE, mon or tetr, I4/m. The structure consists of a framework of octahedrally coordinated metal ions. The octahedra are linked by edge-sharing to form double columns parallel to the tunnel axis. The double strings in turn share corners to form a three-dimensional framework

containing square tunnels. The structure of akaganeite is a modification of the hollandite structure. The octahedral cations are predominantly Fe³⁺, whereas in virtually all other known hollandite-type compounds the octahedra primarily contain tetravalent cations, typically Mn or Ti, and Cl is the major cation tunnel species, as opposed to large univalent or divalent cations such as Ba or K that are typical in most hollandite-type phases.

DEBGA	ANKANGITE	Ba(Ti,V,Cr) ₈ O ₁₆
DEBGB	CORONADITE	Pb(Mn,Mn) ₈ O ₁₆
DEBGC	CRYPTOMELANE	K(Mn,Mn) ₈ O ₁₆
DEBGD	HOLLANDITE	Ba(Mn,Mn) ₈ O ₁₆
DEBGE	MANJIROITE	(Na,K)(Mn,Mn) ₈ O ₁₆ nH ₂ O
DEBGF	MANNARDITE	$Ba(Ti_6V_2)O_{16}$
DEBGG	PRIDERITE	(K,Ba)(Ti,Fe) ₈ O ₁₆
DEBGH	REDLEDGEITE	$BaTi_6Cr_2O_{16}H_2O$
DEBGI	ROMANECHITE	$(Ba,H_2O)(Mn,Mn)_5O_{10} \qquad mon/C2/c$
DEBGJ	FERRIHOLLANDITE	Ba(Fe,Mn) ₈ O ₁₆
DEBGK	STRONTIOMELANE	$SrMn^{4+}{}_{6}Mn^{3+}{}_{2}O_{16}$
DEBGL	HENRYMEYERITE	Ba(Ti ₇ Fe ²⁺)O ₁₆
DEBGM	JEPPEITE	(K,Ba) ₂ (Ti,Fe) ₆ O ₁₃
DEBGN	AKAGANEITE	Fe _{7.6} Ni _{0.4} O _{6.35} (OH) _{9.65} Cl _{1.25}
DEBGO	TODOROKITE	(Mn,Ca,Mg)Mn ₃ O ₇ [·] H ₂ O
DEBGP	FERRICORONADITE	Pb(Mn ⁴⁺ ₆ Fe ³⁺ ₂)O ₁₆
DEPGQ	NIXONITE	Na ₂ Ti ₆ O ₁₃

SERIES H MINIUM, tetr/P4₂/mbc. The structure is based on the packing of Pb^{IVo}O₄ chains, with Pb^{II} ions in the interstices, having 3n coordination. This arrangement is in agreement with the perfect cleavage along the (110) planes, and also with the strong valence of the Pb atoms in these chains. The versiliaite structure is related to schafarzikite by every fourth Sb³⁺ ion in the ψ -tetrahedral chains is substituted by a Fe ion and a sulfide anion is added between two Fe cations in adjacent chains. The corner-sharing Fe tetrahedra connect the chains to build double-chain ribbons.

TRIPPKEITE	CuAs ₂ O ₄	
SCHAFARZIKITE	FeSb ₂ O ₄	
MINIUM	Pb ₂ PbO ₄	
APUANITE	FeFe ₄ Sb ₄ O ₁₂ S	
VERSILIAITE	$Fe_4Fe_8Sb_{12}O_{32}S_2$	Pbam or Pba2
KUSACHIITE	CuBi ₂ O ₄	
	SCHAFARZIKITE MINIUM APUANITE VERSILIAITE	SCHAFARZIKITEFeSb2O4MINIUMPb2PbO4APUANITEFeFe4Sb4O12SVERSILIAITEFe4Fe8Sb12O32S2

SERIES I ALPHA PbO₂, orth/Pbcn. Structure consist of edge-sharing PbO₆ octahedra forming zigzag chains // [001] that are corner-linked to analogous chains, two underlain and two overlain along [100], forming sheets // (100).

DEBIA	SCRUTINYITE	PbO ₂	
DEBIB	SEIFERTITE	SiO ₂	Pbcn/Pb2n

SERIES J ANZAITE-(Ce), mon/C2/m. The structure consists of alternating layers of type 1, populated by REE in an eightfold-coordinated and octahedrally coordinated Fe, and type 2, built of fivefold-and octahedrally coordinated Ti, stacked // to (001). This atomic arrangement is complicated by significant disorder affecting the Fe, fivefold-coordinated Ti and two of the four anion sites. Chakhmouradian, A.R., Cooper, M.A., Medici, L., Abdu, Y.A. and Shelukhina, Y.S. (2013) Anzaite -(Ce), IMA 2013-004. CNMNC Newsletter No. 16, August 2013, page 2701; *Mineralogical Magazine*, **77**, 2695 -2709. DEBJA ANZAITE-(Ce)

Ce₄FeTi₆O₁₈(OH)₂

SERIES K RASPITE, mon/P2₁/a. Structure consists of WO₆ octahedra sharing edges to form zigzag chains // [010]; the chains are linked by Pb atoms.

DEBKA RASPITE PbWO₄

SERIES L COUSINITE, Structure not known. Q/D G.F. Davidson (1954): in Summary of progress Geol. Surv. G. Gr., p.70

J.F. Vaes (1958): "Cousiniet, een nieuw uraanmineral". Geologie en Mijnbouw 20, 449.

American Mineralogist: 44: 910.

M. Deliens (1975): "Une association de molybdates d'uranium de Shinkolobwe (région du Shaba, République du Zaïre)". Annales de la Société Géologique de Belgique 98, 155-160.

M. Deliens & P. Piret (1976): "Nouvelles sonnées sur une umohoite magnésienne de Shinkolobwe (région du Shaba, République du Zaïre)". Annales de la Société Géologique de Belgique 99, 205-209.

DEBLA COUSINITE MgU2⁺⁴Mo2O13⁻⁶H2O

SERIES M ILSEMANNITE, amor. Q/D. Structure not known. Höfer (1871), Jb. Min.: 566.

Horton (1916), US Bureau of Mines Bulletin 111: 15.

Schaller (1917), WashingtonAc Sc., Journal: 7: 417.

Hess (1923), USGS Bulletin 750A.

Palache, Charles, Harry Berman & Clifford Frondel (1944), The System of Mineralogy of James Dwight Dana and Edward Salisbury Dana Yale University 1837-1892, Volume I: Elements, Sulfides, Sulfosalts, Oxides. John Wiley and Sons, Inc., New York. 7th edition, revised and enlarged: 603-604.

Staples, Lloyd William (1951), Ilsemannite and jordisite: American Mineralogist: 36: 609-614.

- DEBMA ILSEMANNITE Mo₃O₈ nH₂O
- SERIES N KUDRYAVTSEVAITE, orth/Pnma. The structure consists of edge-sharing and corner-sharing chains composed of Mg, Fe and Ti atoms coordinated by six atoms of O and running along the b axis, with Na filling the tunnels formed by the chains. Anashkin, S., Bovkun, A., Bindi, L., Garanin, V. and Litvin, Y. (2013) Kudryavtsevaite, IMA 2012-078. CNMNC Newsletter No. 15, February 2013, page 10; Mineralogical Magazine, 77, 1-12.

DEBNA KUDRYAVTSEVAITE Na₃(Mg,Fe)(Fe,Ti)₂Ti₃O₁₂

SERIES O DUMORTIERITE, orth/Pnma. Structure consists three kinds of chains running parallel to <u>a</u>. The first is a partly disordered [AI,TaO₃] chain of face-sharing octahedra; the other two types are [AI₄O₁₂] chains, one of which joins to equivalent chains by reflection at the corners of octahedra to form [AI₄O₁₁] sheets. Dumortierite and magnesiodumortierite constitute a subgroup; holtite, nioboholtite, and titanoholtite constitute a subgroup and szklaryite is the first of a new subgroup.

DEBOA	DUMORTIERITE	Si ₃ B[Al _{6.75} • _{0.25} O _{17.25} (OH) _{0.75}]
DEBOB	MAGNESIODUMORTIERITE	$[Si(Si_{0.94}P_{0.01}\bullet_{0.05})_2O_{15}(OH)_3]B[(Mg,Ti,Fe,\Box)(AI,\Box)(AI,Mg,\Box)_2$
DEBOC	HOLTITE	(AI,Ta,⊡)AI ₆ (BO ₃)(Si,Sb ³⁺ As ³⁺) ₃ O ₁₂ (O,OH,⊡) ₃
DEBOD	NIOBOHOLTITE	(Nb _{0.6} □ _{0.4})Al ₆ BSi ₃ O ₁₈
DEBOE	TITANOHOLTITE	(TiO _{0.75} □ _{0.25})Al ₆ BSi ₃ O ₁₈
DEBOF	SZKLARYITE	$\Box AI_6BAs^{3+}{}_{3}O_{15}$

SERIES P BECKETTITE-ADDIBISCHOFFITE SERIES, <u>Sapphirine Supergroup</u>

DEBPA	BECKETTITE	$Ca_2V_6AI_6O_{20}$
DEBPB	ADDIBISCHOFFITE	Ca ₂ Al ₆ Al ₆ O ₂₀

- SERIES Q BYRUDITE, mon/Pnma. The structure has the norbergite-type and is based on a hexagonal closest packing of O, OH and F, with Mg atoms in octahedral voids forming a zigzag pattern, and Si atoms in tetrahedral voids. The serrated chain of edge-sharing octahedra consists of five unique octahedra. It can be imagined derived from olivine and brucite.
- DEBQA BYRUDITE BeV2⁶⁺O6

GROUP F LAYER STRUCTURES

TYPE A SIMPLE

- SERIES A MOLYBDITE, orth/Pbnm. Structure consists of zigzag chains of edge-sharing MoO₆ octahedra // [001] which are linked by sharing corners of the octahedra.
- DFAAA MOLYBDITE MoO₃
- SERIES B FREUDENBERGITE, mon/C2/m. Structure consists of edge-sharing (Ti,Fe)O₆ octahedra forming double sheets // (001); the sheets are connected into a framework by sharing corners of octahedra in adjoining sheets; cavities in the framework are occupied by Na polyhedra.
- DFABA FREUDENBERGITE Na₂(Ti,Fe)₈O₁₆
- SERIES C BROOKITE, orth/Pbca. The structure is based on a closest packing with a <u>ch</u> sequence, where the Ti atoms are located in one half of the octahedral voids. On the closest packed layers, which are parallel to (100), the Ti atoms form a zigzag pattern. The Ti octahedra share three edges, resulting in zigzag chains with each octahedron sharing one edge with an octahedron of the adjoining chain. In tellurite, dimers of edge-sharing TeO₄ distorted square pyramids sharing corners to form corrugated sheets // (100); in paraqtellurite, similar distorted te square pyramids share corners to form a framework similar to that of cristobalite.
- DFACA BROOKITE TiO₂
- DFACB
 TELLURITE
 TeO2

 DFACC
 PARATELLURITE
 TeO2
 tetr/P41212 or P43212
- SERIES D CLAUDETITE SERIES, mon/P21/n. Structure consists of flat trigonal pyramids of AsO3 sharing O corners to form undulating sheets // (010), with chain-like units // [001].
- DFADA CLAUDETITE As₂O₃ DFADB STIBIOCLAUDETITE AsSbO₃
- SERIES E LITHARGE SERIES, tetr/P4/nmm. Structure consists of PbO₄ square pyramids, with Pb at the apex, sharing edges to form undulating sheets // (001); the sheets are linked by van der Waals bonding.

DFAEA	LITHARGE	PbO
DFAEB	ROMARCHITE	SnO
DFAEC	MASSICOT	PbO (Distorted Litharge Structure)
DFAED	PALLADINITE	PdO tetr.

SERIES F SHAKHOVITE SERIES, mon/ Structure consists of isolated Sb(OH)₃O₃ octahedra which are linked into layers // (010) by H-bonding; these layers are connected by Hg-Hg dimers.

DFAFA	SHAKHOVITE	$(Hg^{+})_{4}(Sb^{5+}O_{3})(OH)_{3}$
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TYPE B COMPLEX

SERIES A EUXENITE SERIES, orth/Pbcn. Structure consists of zigzag chains of edge-sharing MO₆ octahedra // [001], as in scrutinyite, are linked to adjacent chains by sharing corners of octahedra, to form double layers // (100); the double layers are linked by a layer of Y polyhedra.

DFBAA	EUXENITE-(Y)	(Y,Ca,Ce,U,Th)(Nb,Ta,Ti) ₂ O ₆
DFBAB	TANTEUXENITE-(Y)	(Y,Ce,Ca)(Ta,Nb,Ti) ₂ (O,OH) ₆
DFBAC	YTTROCRASITE-(Y)	(Y,Th,Ca,U)(Ti,Fe) ₂ (O,OH) ₆
DFBAD	FERSMITE	(Ca,Ce,Na)(Nb,Te,Ti) ₂ (O,OH,F) ₆
DFBAE	URANOPOLYCRASE	(U,Y)(Ti,Nb) ₂ O ₆
DFBAF	POLYCRASE-(Y)	(Y,U)(Ti,Nb) ₂ O ₆

SERIES B BRANNERITE, mon/C2/m. In brannerite and thorutile, edge-sharing TiO₆ octahedra form zigzag chains // [010] ; the chains are joined into sheets // (001) by sharing edges of octahedra ; the sheets are linked by the large cations in 6 coordination.

DFBBA	BRANNERITE	(U,Ca,Y,Ce)(Ti,Fe) ₂ O ₆
DFBBB	THORUTITE	(Th,U,Ca)Ti ₂ (O,OH) ₆
DFBBC	ORTHOBRANNERITE	$UUTi_4O_{12}(OH)_2$ (orth/)

SERIES C KOECHLINITE, orth/Pna2₁. In koechlinite, sheets of corner-sharing (Mo,W)O₆ octahedra // [010] alternate with sheets of corner-sharing BiO₆ polyhedra; the sheets are linked by shared O atoms.

DFBCA	KOECHLINITE	Bi ₂ MoO ₆	
DFBCB	RUSSELLITE	Bi ₂ WO ₆	
DFBCC	TUNGSTIBITE	Sb ₂ WO ₆	P22 ₁ 2 ₁

SERIES D CREDNERITE, mon/C2/m. Structure consists of edge-sharing M³⁺O₆ octahedra forming sheets // (001); the sheets are linked by linear O-Cu-O groups // [001].

DFBDA CREDNERITE CuMnO₂

SERIES E DELAFOSSITE, trig/R<u>3</u>m. Structure consists of edge-sharing Fe³⁺O₆ octahedra forming sheets // (0001); the sheets are linked by linear O-Cu-O groups; the Cu atoms form a hexagonal array with short Cu-Cu distances.

DFBEA DELAFOSSITE CuFeO₂ DFBEB MCCONNELLITE CuCrO₂

SERIES F CHILUITE, hex/P6₃22, P6₃m or P6₃. Structure not known. May belong in the tellurate group.

DFBFA CHILUITE Bi₆Te₂Mo₂O₂₁

DFBFB SANTANAITE Pb₁₁CrO₁₆

SERIES G ZENZENITE, hex/P6₃/mcm. The structure is of the Pb₃Mn₇O₁₅ type and consists of layers perpendicular to the [001] direction of edge-sharing coordination octahedra around the Mn(Fe) positions. The Pb positions are located between the layers.

DFBGA ZENZENITE Pb₃(Fe,Mn)₄Mn₃O₁₅

SERIES H BAHIANITE, mon/C2/m. Structure consists of sheets // (001) of edge-sharing Al(O,OH)₆ octahedra alternating with linear trimers of edge-sharing Sb⁵⁺O₆ octahedra; the two entities are linked by sharing corners of octahedra.

DFBHA BAHIANITE

SERIES I CARLOSBARBOSAITE, orth/Cmcm. The structure contains a single U site with an appreciable deficiency in electron scattering, which is populated by U atoms and vacancies. The U site is surrounded by seven O atoms in a pentagonal bipyramidal arrangement. The Nb site is coordinated by four O atoms and two OH groups in an octahedral arrangement. The half-occupied tunnel Ca site is coordinated by four O atoms and four water groups. Octahedrally coordinated Nb polyhedra shares edges and corners to form Nb₂O₆(OH)₂ double chains, and edge-sharing pentagonal bipyramidal U polyhedra to form UO₅ chains. The Nb₂O₆(OH)₂ and UO₅ chains share edges to form an open U-Nb -Φ framework with tunnels along [001] that contain Ca(H₂O)₄ clusters. The structure is closely related to a family of synthetic U-Nb-O framework tunnel structures. The structure resembles that of holfertite.

- SERIES J ZIMBABWEITE, orth/Ccmb. The structure has a novel bronze-type, corrugated, corner-linked M(1)₄O₁₈ octahedral sheet made up of four- and eight-membered octahedral rings parallel to (100). Within the octahedral sheet, a large distorted seven-coordinated site, M(3), is occupied by Na. The octahedral sheets are cross-linked by trigonal-pyramidal arsenite groups and trigonal prisms around M(2), which is occupied by (PbNa_{0.5}K_{0.5}).
- DFBJA ZIMBABWEITE Na(Pb,Na,K)₂As₄(Ta,Nb,Ti)₄O₁₈
- SERIES K GREENWOODITE, trig/P<u>3</u>m1. The structure is based on hexagonal closest packing of oxygen atoms with 4 distinct cation layers designated BV, BV1, V2, and V3 having a stacking sequence BV-V1-V2-V3-V2-V1-BV-V1-... the core layers contain 3 distinct V-dominated sites, one tetrahedral Si site and one Fe-dominated tetrahedral site containing a disordered mixture of equal amounts of trivalent and divalent cations. The BV layer is a disordered mixture of 2 endmember layer structures related by the coupled substitution 2Ba = 2O + 2V +1□ + 2H. In the Ba endmember the Ba is at a cubo-octahedral site formed by a hole in one of the hcp oxygen layers. In the VOH endmember the Ba is replaced by an O atom which forms the shared corner of a triplet of octahedral sites.

DFBKA GREENWOODITE Ba_{2-x}(V³⁺OH)_xV₉(Fe³⁺Fe²⁺)₂Si₂O₂₂

- SERIES L CHANGBAIITE, trig/R3m. Structure consists of dimmers of edge-sharing NbO₆ octahedra which are linked into sheets of 6-membered rings // (0001) with Pb in the rings; the sheets are linked by sharing corners of octahedra and by the Pb atoms.
- DFBLA CHANGBAIITE PbNb₂O₆
- SERIES M CHROMBISMITE, tetr/. Structure not known. Zhou Xinchun, Yan Jincai, Wang Guanxin, Wang Shizhong, Liu Liang, and Shu Guiming (1996): A new oxide of bismuth and chromium Chrombismite. Acta Mineralogica Sinica 16(1), 335-339 (in Chinese with English abstract). New Minerals 1995-1999, 48 (abstract).

Zhou Xinchun, Yan Jincai, Wang Guanxin, Wang Shizhong, Liu Liang, and Shu Guiming (1997): Chrombismite, Bi16CrO27, a new mineral species from the Jialu gold mine, Shaanxi Province, China. Canadian Mineralogist 35, 35-38.

Mineralogical Record 28, 484.

- DFBMA CHROMBISMITE Bi₁₆CrO₂₇
- SERIES N BAUMOITE, mon/P2₁/m.
- DFBNA BAUMOITE BaU₃Mo₂O₁₆(H₂O)₆
- SERIES O OPHIRITE, tric/P<u>1</u>. The structural unit in ophirite consist of a [Zn₂Mn₂(H₂O)₂] octahedral layer sandwiched between opposing heteropolytungstate tri-lacunary (FeW₉O₃₄) Keggin anions. Charge balance in the ophirite structure is maintained by the {[Mg9H₂O)₆]₄[Ca(H₂O)₆]₂.10H₂O}¹²⁺ interstitial

DFBIA CARLOSBARBOSAITE (Ca_{0.5}](UO₂)₂(NbSi)O₆(OH)₂.2H₂O

unit. The interstitial unit in the structure of ophirite is formed of two distinct $Mg(H_2O)_6$ octahedra and a Ca(H_2O)₆O₁ polyhedron, as well as five isolated water molecules the linkage between the structural unit and the interstitial unit results principally from H bonding between O atoms of the structural unit with H atoms of the interstitial unit. Ophirite is the first known mineral to contain a lacunary defect derivative of the Keggin anion, a heteropolyanion that is well known in synthetic phase. Kampf, A.R., Hughes, J.M., Marty, J., Nash, B.P. and Wright, S.E. (2013) Ophirite, IMA 2013-017. CNMNC Newsletter No. 16, 2013, page 2704, *Mineralogical Magazine*, **77**, 2695-2709.

Kampf, A.R., Hughes, J.M., Nash, B.P., Wright, S., Rossman, G.R., Marty, J. (2014): Ophirite, Ca2Mg4[Zn2Mn3+2(H2O)2(Fe3+W9O34)2]•46H2O, a new mineral with a heteropolytungstate tri-lacunary Keggin anion. *American Mineralogist*, **99**, 1045-1051.

- DFBOA OPHIRITE (Fe,Zn,Sb)₂(Mn,Zn,Fe,Sb)₂(H₂O)₂(Zn,Fe,Fe,Mn)₂(W,Mg)₁₈O₆₈ Mg(H₂O)₆(Ca,Mn)(H₂O)₆.10H₂O
- SERIES P PAQUEITE, trig/P321. Ma, C. (2013) Paqueite, IMA 2013- 053. CNMNC Newsletter No. 17, October 2013, page 3002; Mineralogical Magazine, 77, 2997- 3005.

DFBPA PAQUEITE Ca₃TiSi₂(Al,Ti,Si)₃O₁₄

SERIES Q NOLLMOTZITE, mon/Cm. Structure consists upon [UV(UO₂)₂F₃O₄]₂ sheets of beta-U₃O₈ topology and contains an interlayer with MgF₂(H₂O)₄.

DFBQA NOLLMOTZITE $Mg[U^{5+}V(U^{6+}O_2)_2O_4F_3].4H_2O$

Updated 05/20/19