

HALIDES

CLASS G	HALIDES	
GROUP A	COORDINATION STRUCTURES	
TYPE A	ANHYDROUS HALIDES	
SERIES A	HALITE SERIES, cubic/Fm3m. The structure is formed by the closest packing of Cl⁻ anions in cubic closest packing with Na⁺ cations occupying all the octahedral interstices.	
GAAAA	HALITE	NaCl
GAAAB	SYLVITE	KCl
GAAAC	VILLIAUMITE	NaF
GAAAD	CAROBBIITE	KF
GAAAE	SALAMMONIAC	NH ₄ Cl
GAAAF	CHLORARGYRITE	AgCl
GAAAG	BROMARGYRITE	AgBr
GAAAH	GRICEITE	LiF
GAAAI	LAFOSSAITE	Tl(Cl,Br)
SERIES B	SPHALERITE Structure type, cubic/F43m.	
GAABA	NANTOKITE	CuCl
GAABB	MIERSITE	(Ag,Cu)I
GAABC	MARSHITE	CuI
SERIES C	WURTZITE Structure type, hex/P6₃mc.	
GAACA	IODARGYRITE	AgI
SERIES D	FLUORITE SERIES, cub/Fm3m. The 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.	
GAADA	FLUORITE	CaF ₂
GAADB	FRANKDICKSONITE	BaF ₂
GAADC	HALENIUSITE-(La)	(La,Ce)OF
GAADD	STRONTIOFLUORITE	SrF ₂
GAADE	FLUOROCRONITE	PbF ₂
SERIES E	COTUNNITE, orth/Pmnb. Cotunnite group. In cotunnite, Pb polyhedra share Cl-Cl edges to form chains // [001] that are linked into sheets // (010); Pb-Cl bonding between sheets. There is a structural, morphological and physical relationship to laurionite in the orientation Pcmn. In barstowite, cotunnite-type sheets alternate with Pb (CO₃).H₂O sheets along [100]. The structure of barstowite can be described in terms of three layers stacked along [001] in the sequence ...CACBCACBC... to give a 16.7 S repeat. Layer A consists of face-sharing PbCl₆ distorted square antiprisms. Layer B is composed of Pb coordinated to 5 Cl and 2 O each with two H to form water groups. Layer C is formed by Pb coordinated to 5 Cl and 3 O which are from carbonate groups. The H positions are deduced and are H-bonded to O from the carbonates.	
GAAEA	COTUNNITE	PbCl ₂
GAAEB	BARSTOWITE	PbCO ₃ ·3PbCl ₂ ·H ₂ O
GAAEC	PSEUDOCOTUNNITE	K ₂ PbCl ₄
GAAED	COCCINITE (?) (G)	HgI ₂

SERIES F **GAGARINITE SERIES, trig/R3 or R₃.** The structure is a stuffed derivative of the UCl₃ arrangement. The Ca,REE atoms are coordinated in a tricapped trigonal prism. The cations bond to three F atoms in the mirror plane above and below 2.366 Å, and also form bonds with three coplanar F atoms through the prism faces.

GAAFA	GAGARINITE-(Y)	NaCaY(F,Cl) ₆
GAAFB	GAGARINITE-(Ce)	NaCaCe(F,Cl) ₆
GAAFC	POIEZHAEVAITE-(Ce)	NaSrCeF ₆

SERIES G **LAURELITE, hex/ P6₃.** The structure is related to αPbF₂. Both are based upon nine-fold coordination Pb as tricapped trigonal prisms (TCTPs), which share edges and faces. The two structures can be described with respect to the face-sharing linkages of their TCTPs. The structure of alpha PbF₂ consists of corrugated sheets of face-sharing TCTPs that interlock by edge-sharing perpendicular to the c axis. In laurelite, the Pb(2) TCTPs form three-membered face-sharing clusters about the threefold axis that are propagated into trigonal cylinders by sharing faces in the direction of the c axis. The Pb(1) and Pb(3) TCTPs are linked by face-sharing into a three-dimensional framework with corresponding cylindrical voids. Asymmetric co-ordinations about Pb(1) and Pb(2) are attributed to the stereoactive lone-pair effect.

GAAGA	LAURELITE	Pb ₇ F ₁₂ Cl ₂
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SERIES H **CHALLACOLLOITE SERIES, mon/P2₁/c. Structure consists of... :**

J. Schlüter, D. Pohl and S. Britvin (2005): The new mineral challacolloite, KPb₂Cl₅, the natural occurrence of a technically known laser material. N. Jb. Min. Abh. 182, 95-101.

Mitolo D., Pinto D., Garavelli A., Bindi L. & Vurro F. (2009): The role of the minor substitutions in the crystal structure of natural challacolloite, KPb₂Cl₅, and hephaistosite, TIPb₂Cl₅, from Vulcano (Aeolian Archipelago, Italy). Mineralogy and Petrology 96, 121-128. Campostrini, I., Demartin, F., Gramaccioli, C.M., Orlandi, P. (2008): Hephaistosite, TIPb₂Cl₅, a new thallium mineral from La Fossa crater, Vulcano, Aeolian Islands, Italy. Canadian Mineralogist, 46, 701-708.

Mitolo D., Pinto D., Garavelli A., Bindi L. & Vurro F. (2009): The role of the minor substitutions in the crystal structure of natural challacolloite, KPb₂Cl₅, and hephaistosite, TIPb₂Cl₅, from Vulcano (Aeolian Archipelago, Italy). Mineralogy and Petrology 96, 121-128.

GAAHA	CHALLACOLLOITE	KPb ₂ Cl ₅
GAAHB	HEPHAISTOSITE	TIPb ₂ Cl ₅

SERIES I **FLINTEITE, orth/Pna21.** The structure contains three Zn sites centering isolated tetrahedra ZnCl₄ tetrahedra and six independent K sites.

GAAIA	FLINTEITE	K ₂ ZnCl ₄
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SERIES J **GRANDREEFITE, orth/I222, F222.** The structure consists of layer fragments of the beta-PbF₂ structure parallel to (100) alternating with layers of isolated sulfate tetrahedra. The layer sequence in the unit cell is SO₄-PbF₂Pb-SO₄-PbF₂Pb-SO₄. Pb is coordinated to four F and four O forming a distorted bicapped trigonal prism. The structure is closely related to that of the lanthanide oxide sulfates, Ln₂O₂SO₄.

GAAJA	GRANDREEFITE	Pb ₂ (SO ₄)F ₂
GAAJB	PSEUDOGRANDREEFITE	Pb ₆ (SO ₄)F ₁₀
GAAJC	SUNDIUSITE	Pb ₁₀ [Cl ₂ /O ₈ /SO ₄]

SERIES K **PANICHIITE, cubic/Fm3m.** Demartin, F., Campostrini, I. & Gramaccioli, C. M. (2009): Panichiite, natural ammonium hexachlorostannate(IV), (NH₄)₂SnCl₆, from La Fossa crater, Vulcano, Aeolian Islands, Italy. Canadian Mineralogist 47, 367-372.

GAAKA	PANICHIITE	(NH ₄) ₂ SnCl ₆
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SERIES L **CHLOROCALCITE, orth, ps cub/. Structure not known. Has the perovskite structure.** Monticelli, T. and Covelli, N. (1823) Storia di fenom. Del Vesuvio avven. Negli anni, 1821, etc., Naples: 183.
Beudant, F.S. (1832), Traité élémentaire de Minéralogie, second edition, 2 volumes: 2: 512.
Scacchi (1872) Reale accademia delle scienze fisiche e matematiche, Naples, Rend., October 12, 1872).

Scacchi (1873) Reale accademia delle scienze fisiche e matematiche, Naples, Mem.: Dec. 13, 1873.

Lacroix (1907) Bulletin de la Société française de Minéralogie: 30: 255.

Zambonini, Ferruccio (1910) Mineralogia Vesuviana. 368 pp., Naples: 50.

Renner (1912) Centralblatt für Mineralogie, Geologie und Paleontologie, Stuttgart: 106 (as Baeumlerite).

Zambonini, Ferruccio (1912) Mineralogia Vesuviana, appendix, 51 pp.: 3.

Zambonini, Ferruccio (1935) Mineralogia Vesuviana, second edition with Quercigh, 463 pp., Naples: 99.

Palache, Charles, Harry Berman & Clifford Frondel (1951), The System of Mineralogy of James Dwight Dana and Edward Salisbury Dana Yale University 1837-1892, Seventh edition, Volume II: 91-92.

GAALA CHLOROCALCITE KCaCl_3

GAALB JAVORIEITE KFeCl_3

SERIES M **ARGESITE, trig/R3c.** Demartin, F., Campostrini, I., Castellano, C. and Gramaccioli, C.M. (2011): Argesite, IMA 2011-072. CNMNC Newsletter No. 11, December 2011, page 2892; Mineralogical Magazine, 75, 2887-2893.

Demartin, F., Campostrini, I., Castellano, C. and Gramaccioli, C.M. (2012): Argesite, $(\text{NH}_4)_7\text{Bi}_3\text{Cl}_{16}$, a new mineral from La Fossa Crater, Vulcano, Aeolian Islands, Italy: a first example of the $[\text{Bi}_2\text{Cl}_{10}]_4^-$ anion. American Mineralogist, 97, 1446-1451.

GAAMA ARGESITE $(\text{NH}_4)_7\text{Bi}_3\text{Cl}_{16}$

SERIES N **SANGUITE, mon/P2₁/c. NH_4CdCl_3 structure. The structure contains almost planar, discrete dimers $[\text{Cu}^{2+}_2\text{Cl}_6]$. The KCl_9 polyhedra are connected via common faces to form interrupted layers. Neighboring layers are linked to each other by the common edges of the K-centered polyhedra.**

Willett, Roger D.; Dwiggins, Claudius, Jr.; Kruh, R. F.; Rundle, R. E. (1963): Crystal Structures of KCuCl_3 and NH_4CuCl_3 . *Journal of Chemical Physics*, 38, 2429-2436

Pekov, I.V., Zubkova, N.V., Belakovskiy, D.I., Lykova, I.S., Vigasina, M.F., Sidorov, E.G. and Pushcharovsky, D.Y. (2013) Sanguite, IMA 2013-002. CNMNC Newsletter No. 16, August 2013, page 2701; *Mineralogical Magazine*, 77, 2695- 2709.

GAANA SANGUITE KCuCl_3

SERIES O **open**

SERIES P **NATALIYAMALIKITE, orth/Cmcm.**

GAAPA NATALIYAMALIKITE TlI

TYPE B **HYDROUS HALIDES**

SERIES A **BISCHOFITE, mon/C2/m. The structure is based on distinct $\text{Mg}(\text{H}_2\text{O})_6\text{Cl}_2$ groups formed by $\text{Mg}(\text{H}_2\text{O})_6$ octahedra, with Cl located at the octahedron faces above and below. Six Cl atoms not in this group form a ring in a plane perpendicular to the axis of the molecule. Structure consists of $\text{Mg}(\text{H}_2\text{O})_6$ octahedra connected into a framework by Cl ions.**

GABAA BISCHOFITE $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$

GABAB ROKUHNITE $\text{FeCl}_2 \cdot 6\text{H}_2\text{O}$

SERIES B	NICKELBISCHOFITE. Structure consists of $\text{Ni}(\text{H}_2\text{O})_4\text{Cl}_2$ pseudo-octahedra which are linked by H-bonding to form sheets // (001); it is not structurally related to bischofite.		
GABBA	NICKELBISCHOFITE	$\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$	
SERIES C	ANTARCTICITE, trig/P321. Structure consists of a framework of $\text{Ca}(\text{H}_2\text{O})_7$ polyhedra linked by Cl atoms.		
GABCA	ANTARCTICITE	$\text{CaCl}_2 \cdot 6\text{H}_2\text{O}$	
SERIES D	ERIOCHALCITE, orth/Pbmn. Structure consists of distorted $\text{CuCl}_2(\text{H}_2\text{O})_4$ octahedra sharing Cl-Cl edges to form linear chains // [001]; the chains are linked by H-bonding from the water molecules.		
GABDA	ERIOCHALCITE	$\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$	
SERIES E	SINJARITE, tetr/. Structure not known. American Mineralogist (1980): 65: 1069. Mineralogical Magazine: 43: 643-645.		
GABEA	SINJARITE	$\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$	
SERIES F	CHLORALUMINITE, trig/R$\bar{3}$c. Structure consists of a framework of insular $\text{Al}(\text{H}_2\text{O})_6$ octahedra linked by Cl atoms.		
GABFA	CHLORALUMINITE	$\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$	
SERIES G	ATACAMITE SERIES. Four polymorphs; three with gibbsite-like sheets of edge-sharing $\text{Cu}(\text{OH})_4\text{Cl}_2$ octahedra – atacamite with sheets // [110], clinoatacamite // (101), and paratacamite // (0001); the sheets are connected by single Cu octahedra, the fourth polymorph, botallackite, has brucite-like sheets // (001) of edge-sharing $\text{Cu}(\text{OH})_4\text{Cl}_2$ octahedra, connected by H-bonding. Botallackite structure consists of sheets of edge-sharing $\text{Cu}\phi_6$ octahedra of composition $\text{Cu}_2(\text{OH})_3\text{Cl}$; these sheets are parallel to {100}, and are joined by H bonding between O and Cl anions, accounting for the perfect {100} cleavage and platy habit. The clinoatacamite structure consists of layers of partly occupied, edge-sharing octahedra of Jahn-Teller-distorted $[\text{Cu}(\text{OH})_4\text{Cl}_2]$ octahedra parallel to (101). This layer is topologically the same as that in mica. Adjacent layers of octahedra are offset, such that vacant sites in one sheet align with occupied sites in the neighboring sheet. Layers are linked by individual, slightly Jahn-Teller distorted octahedra of composition $[\text{Cu}(\text{OH})_6]$. The structures of paratacamite and the other polymorphs of $\text{Cu}_2(\text{OH})_3\text{Cl}$, atacamite and botallackite, also are layered, but they differ from the layering of clinoatacamite in topology, composition and cross-linkage. The structure of kapellasite and its Mg analogue consists of sheets made from edge-sharing $\text{Cu}(\text{OH})_4\text{Cl}_2$ and $\text{Zn}(\text{OH})_6$ octahedra. The sheets are only weakly linked by O-H-Cl bridges, giving rise to perfect cleavage along (001) and to strong texture effects in powder diffraction data. Kuliginite can be regarded as the Fe-analog of tonidiite. The crystal structure has atomic packing similar to spinel structure with vacant tetrahedral sites. See AM 103, 1435 for more detailed description.		
	F. C. Hawthorne, M. A. Cooper, J. D. Grice, A. C. Roberts & N. Hubbard (2002): Description and crystal structure of bobkingite, $\text{Cu}_2+5\text{Cl}_2(\text{OH})_8(\text{H}_2\text{O})_2$, a new mineral from New Cliffe Hill Quarry, Stanton-under-Bardon, Leicestershire, UK. Mineralogical Magazine: 66, 301-311.		
GABGA	ATACAMITE	$\text{Cu}_2(\text{OH})_3\text{Cl}$	orth/Pmcn
GABGB	KEMPITE	$\text{Mn}_2(\text{OH})_3\text{Cl}$	orth/Pnam
GABGC	PARATACAMITE	$\text{Cu}_2(\text{OH})_3\text{Cl}$	trig/R $\bar{3}$
GABGD	BOTALLACKITE	$\text{Cu}_2(\text{OH})_3\text{Cl}$	mon/P2 $_1$ /m
GABGE	HIBBINGITE	$\gamma\text{-Fe}_2(\text{OH})_3\text{Cl}$	orth/Pnam
GABGF	CLINOATACAMITE	$\text{Cu}_2(\text{OH})_3\text{Cl}$	mon/P2 $_1$ /n

GABGG	BELLOITE	$\text{Cu}(\text{OH})\text{Cl}$	mon/P2 ₁ /a
GABGH	HERBERTSMITHITE	$\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$	trig/R3m
GABGI	KAPELLASITE	$\text{Cu}_3\text{Zn}(\text{OH})_6\text{Cl}_2$	trig/P3m1
GABGJ	AVDONINITE	$\text{K}_2\text{Cu}_5[(\text{OH})_4\text{Cl}_8]\cdot\text{H}_2\text{O}$	mon/P2/m, Pm, or P2
GABGK	HAYDEEITE	$\text{Cu}_3\text{MgCl}_2(\text{OH})_6$	Trig/P3m1
GABGL	GILLARDITE	$\text{Cu}_3\text{NiCl}_2(\text{OH})_6$	Trig/R3m
GABGM	KULIGINITE	$\text{Fe}_3\text{Mg}(\text{OH})_6\text{Cl}_2$	Trig/R3
GABGN	LEVERETTITE	$\text{Cu}_3\text{CoCl}_2(\text{OH})_6$	trig/R3m
GABGO	PARATACAMITE-(Mg)	$\text{Cu}_3(\text{Mg,Cu})\text{Cl}_2(\text{OH})_6$	trig/R3
GABGP	PARATACAMITE-(Ni)	$\text{Cu}_3(\text{Ni,Cu})\text{Cl}_2(\text{OH})_6$	trig/R3
GABGQ	TONDIITE	$\text{Cu}_3\text{MgCl}_2(\text{OH})_6$	trig/R3
GABGR	CENTENNIALITE	$\text{CaCu}_3\text{Cl}_2(\text{OH})_6\cdot n\text{H}_2\text{O}$	trig/P3
GABGS	IYOITE	$\text{MnCuCl}(\text{OH})_3$	mon/P2 ₁ /m
GABGT	MISAKIITE	$\text{Cu}_3\text{Mn}(\text{OH})_6\text{Cl}_2$	trig/P3m1
GABGU	IYOITE	$\text{MnCuCl}(\text{OH})_3$	mon/P2 ₁ /m
GABGV	MISAKIITE	$\text{Cu}_3\text{Mn}(\text{OH})_6\text{Cl}_2$	trig/P3m1
GABGW	BOBKINGITE	$\text{Cu}_5\text{Cl}_2(\text{OH})_8(\text{H}_2\text{O})_2$	mon/C2/m

SERIES H **BOLEITE SERIES, cub & tet.** The structure (cumengite) can best be described as a rod structure, with each rod centered on a 4-fold axis in the unit cell. The Pb(1)Cl₆ octahedron lies on the 4-fold axis at the origin of the unit cell, and is surrounded by a double-tiered necklace of edge-sharing Cu(1)(OH)₄Cl₂ octahedra embedded in the outside of the necklace and promoting linkage between the upper and lower tiers in the Cu(2)(OH)₄Cl square pyramid. This compact unit links upwards to another compact unit centered on the Pb(2)Cl₈ square antiprism. The lower section of this unit is the 4-membered ring of corner-sharing Pb(3)Cl₆(OH) augmented trigonal prisms. These rods form a body-centered array, and share polyhedral edges and corners to form a continuous 3-dimensional structure.

GABHA	BOLEITE	$\text{Pb}_{26}\text{Ag}_9\text{Cu}_{24}(\text{OH})_{48}\text{Cl}_{62}$	cub/Pm3m
GABHB	BIDEAUXITE	$\text{Pb}_2\text{Ag}(\text{F,OH})_2\text{Cl}_3$	cub/Fd3m
GABHC	CUMENGITE	$\text{Pb}_{21}\text{Cu}_{20}(\text{OH})_{40}\text{Cl}_{42}$	tetr/I4/mmm
GABHD	PSEUDOBOLEITE	$\text{Pb}_5\text{Cu}_4(\text{OH})_8\text{Cl}_{10}\cdot 2\text{H}_2\text{O}$	tetr/I4/mmm

SERIES I **CARNALLITE, orth/Pbnn.** The structure consists of a network of face-sharing KCl₆ octahedra linked to Mg(H₂O)₆ octahedra occupying the openings in the KCl network. The water molecules act as charge transmitters between Mg and Cl ions. Structure consists of dimers of face-sharing KCl₆ octahedra sharing corners with a monomeric KCl₆ octahedron to form a 3-dimensional framework. Large cavities in the framework accommodate Mg(H₂O)₆ octahedra which have a coordination of 12 with respect to Cl. Okrugin, V.M., Kudaeva, S.S., Karimova, O.V., Yakubovich, O.V., Belakovskiy, D.I., Chukanov, N.V., Zolotarev, A.A., Gurzhiy, V.V., Zinovieva, N.G., Shiryaev, A.A., Pavel M. Kartashov, P.M. (2019): The new mineral novograbenovite, (NH₄,K)MgCl₃·6H₂O from the Tolbachik volcano, Kamchatka, Russia: mineral information and crystal structure. Mineralogical Magazine, 83, 223-231.

Abstract:

The new mineral novograbenovite, (NH₄,K)MgCl₃·6H₂O, was found on basaltic lava from the 2012–2013 Tolbachik fissure eruption at the Plosky Tolbachik volcano, Kamchatka Peninsula, Russia. It occurs as prismatic, needle-like transparent crystals together with gypsum and halite. Novograbenovite was formed due to the exposure of the host rocks to eruptive gas exhalations enriched in HCl and NH₃. Basalt was the source of potassium and magnesium for the mineral formation. Novograbenovite crystallises in the monoclinic space group C2/c, with unit-cell parameters a = 9.2734(3) Å, b = 9.5176(3) Å, c = 13.2439(4) Å, β = 90.187(2)°, V = 1168.91(2) Å³ and Z = 4. The five strongest reflections in the powder X-ray diffraction pattern [dobs, Å (I, %) (h k l)] are: 3.330 (100) (2 2 0), 2.976 (45) (-114), 2.353 (29) (-224), 3.825 (26) (2 0 2), 1.997 (25) (-4-22). The density

calculated from the empirical formula and the X-ray data is 1.504 g cm⁻³. The mineral is biaxial (+) with $\alpha = 1.469(2)$, $\beta = 1.479(2)$ and $\gamma = 1.496(2)$ ($\lambda = 589$ nm); $2V_{\text{meas.}} = 80(10)^\circ$ and $2V_{\text{calc.}} = 75.7^\circ$. The crystal structure (solved and refined using single-crystal X-ray diffraction data, $R1 = 0.0423$) is based on the perovskite-like network of (NH₄,K)Cl₆-octahedra sharing chlorine vertices, and comprises [Mg(H₂O)₆]²⁺ groups in framework channels. The positions of all independent H atoms were obtained by difference-Fourier techniques and refined isotropically. All oxygen, nitrogen and chlorine atoms are involved in the system of hydrogen bonding, acting as donors or acceptors. The formula resulting from the structure refinement is [(NH₄)_{0.7}K_{0.3}]MgCl₃·6H₂O. The mineral is named after Prokopyi Trifonovich Novograbenov, one of the researchers of Kamchatka Peninsula, a teacher, naturalist, geographer and geologist.

GABIA	CARNALLITE	KMgCl ₃ ·6H ₂ O
GABIB	NOVOGRABLENOVITE	(NH ₄ ,K)MgCl ₃ ·6H ₂ O
SERIES J	TACHYHYDRITE, trig/R$\bar{3}$c. Structure consists of insular CaCl ₆ and two Mg(H ₂ O) ₆ octahedra which are linked into a 3-dimensional framework by H-bonding.	
GABJA	TACHYHYDRITE	Mg ₂ CaCl ₆ ·12H ₂ O
SERIES K	MITSCHERLICHITE, tetr/P4₂/mnm. Structure consists of a framework of KCl ₈ cubes and CuCl.	
GABKA	MITSCHERLICHITE	K ₂ CuCl ₄ ·2H ₂ O
SERIES L	ZIRKLERITE, trig/. Structure not known. Kali, Halle (1928), 22, 157-161. American Mineralogist (1928): 13: 592. Palache, Charles, Harry Berman & Clifford Frondel (1951), The System of Mineralogy of James Dwight Dana and Edward Salisbury Dana Yale University 1837-1892, Seventh edition, Volume II: 87.	
GABLA	ZIRKLERITE Q/D	(Fe,Mg,Ca) ₉ Al ₄ Cl ₁₈ (OH) ₁₂ ·14H ₂ O?
SERIES M	FEODOSIYITE, mon/P2₁/c. The structure is based on layers of Cu ²⁺ - centered polyhedra. Cu ²⁺ cations occupy six crystallographically non-equivalent sites that are placed in distorted octahedra and distorted tetragonal pyramids. Isolated almost regular Mg(H ₂ O) ₆ octahedra, linked with the layers of Cu-centered polyhedra by H-bonds, occur in the interlayer space, as well as separate water molecules.	
GABMA	FEODOSIYITE	Cu ₁₁ Mg ₂ Cl ₁₈ (OH) ₈ ·16H ₂ O
SERIES N	HYDROHALITE, mon/P2₁/c. Structure consists of edge-sharing NaCl ₂ (H ₂ O) ₄ octahedra forming sheets // (100) similar to those in gibbsite. H-bonding between the sheets.	
GABNA	HYDROHALITE	NaCl · 2H ₂ O
SERIES O	GHIARAITE, tric/P$\bar{1}$. The structure consists of the Ca ion to be coordinated by 3 Cl ⁻ + 4H ₂ O, forming Ca ₂ Cl ₄ (H ₂ O) ₈ molecular moieties that are held together by only weak H-bonds and van der Waals forces.	
GABOA	GHIARAITE	CaCl ₂ ·4H ₂ O
SERIES P	CYROBOSTRYXITE, mon/P2₁/c. The structure contains isolated Zn-centered tetrahedra ZnCl ₃ (H ₂ O) connected via eight-coordinated K-centered polyhedra KCl ₇ (H ₂ O) to form a pseudo-framework. Both Zn- and K-centered polyhedra involve only O(1) atoms of the H ₂ O(1) molecules, whereas H ₂ O(2) molecules are located in holes of the K-Zn-Cl-H ₂ O(1) polyhedra pseudo-framework. Pekov, I.V., Zubkova, N.V., Britvin, S.N., Yapaskurt, V.O., Chukanov, N.V., Lykova, I.S., Sidorov, E.G. and Pushcharovsky, D.Y. (2014) Cryobostryxite, IMA 2014-058. CNMNC Newsletter No. 22, October 2014, page 1247; <i>Mineralogical Magazine</i> , 78 , 1241-1248.	
GABPA	CYROBOSTRYXITE	KZnCl ₃ ·2H ₂ O

SERIES Q CABVINITE, tetr/14/m. Structure consists of Th tricapped trigonal prisms, connected through corner-sharing, giving rise to a framework hosting [001] tunnels.

GABQA CABVINITE $\text{Th}_2\text{F}_7(\text{OH})\cdot 3\text{H}_2\text{O}$

GROUP B FRAMEWORK STRUCTURES

TYPE A ANHYDROUS HALIDES

SERIES A PEROVSKITE Structure type, 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. The diabolite structure may be described as a defect-perovskite arrangement of the form $\text{Pb}_2(\text{Cu}^\bullet)\text{O}_6$ in which half of the octahedra are not occupied by cations. The structure consists of a sheet of isolated Cu octahedra at the nodes of a 4_4 net. This arrangement is repeated in the [001] direction by the lattice translation to form corner-sharing $[\text{Cu}^{2+}\text{O}_5]$ chains parallel to [001].

GBAAA NEIGHBORITE NaMgF_3

GBAAB DIABOLEITE $\text{Pb}_2\text{Cu}(\text{OH})_4\text{Cl}_2$ tetr/P4mm, defective perovskite structure

SERIES B GANANITE, cub/P43m. Structure consists of atoms having eight nearest neighbors; the coordination spheres are BiF_8 , FF_8 and $\text{F}(\text{Bi}_4\text{F}_4)$.

GBABA GANANITE BiF_3

SERIES C TVEITITE, trig/R3 or $R\bar{3}$. Structure based on that of fluorite, with the addition of five extra F atoms per formula unit, resulting in clusters of 13 cubic close-packed F ions; six YF_{8+1} monocapped square prisms share on F atom to form Y_6F_{13} clusters; the clusters are connected into columns // [0001] by CaF_{12} polyhedra; the clusters are embedded in a fluorite-type structure. The defect new structure of the mineral manifests itself in a mixed occupation of all four independent cation positions and in a randomly disordered distribution of fluorine atoms over the majority of anion positions.

GBACA TVEITITE-(Y) $(\text{Y},\text{Na})_6(\text{Ca},\text{LREE})_6(\text{Ca},\text{Na},\text{HREE})_6(\text{Ca},\text{Na})\text{F}_{42}$

SERIES D VASILYEVITE, tric/P1. The structure consists of strongly bonded [X-Hg-Hg-X] tetramers. These groups link together at their anion vertices to form a complex interpenetrating framework of two discrete three- and four-connecting nets. The halogen atoms and the carbonate and sulfur anions occur in the interstices of the two nets and serve to stabilize the nets via additional weak linkages to Hg atoms. The structure most resembles the structures of poyarkovite and eglestonite.

GBADA VASILYEVITE $(\text{Hg}_2)^{2+}_{10}\text{O}_6\text{I}_3\text{Br}_2\text{Cl}(\text{CO}_3,\text{S})$

SERIES E open

SERIES F OSKARSSONITE, rhom/R3c. The structure can be described as a rhombohedral deformation of the idealized cubic perovskite-type octahedral framework of corner-sharing AlF_6 groups.

GBAFA OSKARSSONITE AlF_3

SERIES G WAIMIRITE, orth,Pnma. The mineral is isomorphous with synthetic SmF_3 , HoF_3 and YbF_3 . The Y atom forms a 9-coordinated YF_9 tricapped trigonal prism in the structure. Has the B-site vacant perovskite structure. Minuzzii, O.R.R., Ferroni, J.M.T.M., Bastos Neto, A.C. & Pereira, V. P. (2003) : Primeira Notícia da Descoberta de Waimirite e Atroarita, Dois Novos Minerais na Mina de Pitinga, AM, Brasil. *Pesquisas em Geociências*, **30** (1): 99-101 <http://www.ufrgs.br/igeo/pesquisas/3001/07-3001.pdf>

Bastos Neto, A.C., Pereira, V.P., Atencio, D., Ferron, J.T.M.M. and Coutinho, J.M.V. (2014) Waimirite-(Y), IMA 2013-108. CNMNC Newsletter No. 19, February 2014, page 167; *Mineralogical Magazine*, **78**, 165-170.

Atencio D, C. Bastos Neto A, P. Pereira V, T.M.M. Ferron J, M.V. Coutinho J, B. Andrade M, Domanik K (2014): Waimirite-(Y), orthorhombic YF_3 from Pitinga Mine, Presidente Figueiredo, Amazonas, Brazil. 21st General Meeting of the IMA (IMA2014), Gauteng, South Africa, September 1-5; Abstract Volume, 372.

GBAGA	WAIMIRITE-(Y)	YF_3
TYPE B	HYDROUS HALIDES	
SERIES A	ABHURITE, trig/R32. Open sheets of Sn trigonal pyramids and dipyramids // (0001) are linked by sheets of Cl ions.	
GBBAA	ABHURITE	$Sn_3O(OH)_2Cl_2$
SERIES B	CADWALADERITE, cub?/ (amor) Structure not known. Gordon (1941) Academy of Natural Science of Philadelphia, Notulae Naturae, no. 80, April, 1941.	
	American Mineralogist (1942): 27: 144.	
	Palache, Charles, Harry Berman & Clifford Frondel (1951), The System of Mineralogy of James Dwight Dana and Edward Salisbury Dana Yale University 1837-1892, Seventh edition, Volume II: 77.	
GBBBA	CADWALADERITE	$Al_5(H_2O)_3(OH)_{12-n}(Cl, H_2O)$
SERIES C	open	
SERIES D	DIOSKOURIITE, mon/orth. 2m, 2O	
GBBCA	DIOSKOURIITE	$CaCu_4Cl_2(OH)_4 \cdot 4H_2O$
SERIES E	SIIDRAITE, orth/Fddd. The structure is based upon a cubane-like $Pb_4(OH)_4$ nucleus that is coordinated to sixteen iodide ions. Cu^+ ions are inserted into pairs of adjacent edge-sharing tetrahedral sites in the iodide motif to form $[Cu_2I_6]^{4-}$ groups. The structure is based upon a cubane-like $Pb_4(OH)_4$ nucleus that is coordinated to sixteen iodide ions. Cu^+ ions are inserted into pairs of adjacent edge-sharing tetrahedral sites in the iodide motif to form $[Cu_2I_6]^{4-}$ groups. The structure of siidraite is a framework comprising an alternation of two structural elements, a cubane-like $[Pb_4(OH)_4]^{4+}$ group and a $[Cu_2I_6]^{4-}$ dimer of edge-sharing CuI_4 tetrahedra with non-equivalent Cu. Six halocuprate groups surround each $[Pb_4(OH)_4]^{4+}$ nucleus, and each halocuprate group is shared between six adjacent $[Pb_4(OH)_4]^{4+}$ groups, five long Pb-I bonds are required to complete the coordination of each Pb atom. The resulting $Pb(OH)_3I_5$ polyhedra are centered on a tetrahedron of O atoms to form a $Pb_4(OH)_4I_{16}$ cluster.	
GBBEA	SIIDRAITE	$Pb_2Cu(OH)_2I_3$
GROUP C	RING STRUCTURES	
GROUP D	INSULAR STRUCTURES	
TYPE A	ANHYDROUS HALIDES	
SERIES A	BARITE Structure type, orth/Pnma. The structure consists of isolated BF_4 tetrahedra linked by M atoms with 12 coordination about the oxygen atoms. This arrangement results in a perfect (001) cleavage.	
GDAAA	AVOGADRITE	$(K, Cs)BF_4$
GDAAB	BARBERIITE	NH_4BF_4
SERIES B	FERRUCCITE (Anhydrite structure type), orth/Cmcm. Structure consists of Na in [4+4] coordination in a 12-faced polyhedron; chains // [100] are formed by edge-sharing of these polyhedra with BF_4 tetrahedra; the chains are connected into a 3-dimensional framework by edge- and corner-sharing with neighboring chains.	
GDABA	FERRUCCITE	$NaBF_4$

SERIES C	PEROVSKITE DERIVATIVE Structures, cub/Fm3m. The structure of hieratite is based on a mixed cubic closest packing of F and K atoms, with the Si atoms occupying 1/8 of the octahedral voids. It may also be imagined as a subtraction interstitial derivative of the perovskite structure.		
GDACA	HIERATITE	K_2SiF_6	
GDACB	CRYPTOHALITE	$(NH_4)_2SiF_6$	
GDACC	DEMARTINITE	$K_2[SiF_6]$	
SERIES D	RINNEITE, trig/R3c. In rinneite, face-sharing $FeCl_6$ and $NaCl_6$ octahedra alternate in chains // [0001], which are cross-linked by 3K. In chlormanganokalite, $FeCl_6$ is replaced by $MnCl_6$ and Na in the chains by K.		
GDADA	RINNEITE	$K_3NaFeCl_6$	
GDADB	CHLORMANGANOKALITE	K_2MnCl_6	
GDADC	SALTONSEAITE	$K_3NaMnCl_6$	
SERIES E	MALLADRITE, trig/P321. Structure consists of groups of three edge-sharing NaF_6 octahedra and one SiF_6 octahedron lie in the (0001) plane, and are linked into sheets // (0001) by F-F bonding; intersheet linkage is by van der Waals forces.		
GDAEA	MALLADRITE	Na_2SiF_6	
GDAEB	BARARITE	$(NH_4)_2SiF_6$	trig/R3m
SERIES F	KNASIBFITE, orth/Imm2. The asymmetric structure unit contains two twelve-coordinated independent K ions, located on <i>m</i> and on <i>mm2</i> sites, respectively, two independent Na ions, of which one is nine-coordinated and the other one displays instead octahedral coordination. Three are also two crystallographically independent octahedral SiF_6^{2-} anions and a tetrahedral BF_4^- anion.		
GDAFA	KNASIBFITE	$K_3Na_4[SiF_6]_3[BF_4]$	
SERIES G	STEROPESITE, mon/Cc. Demartin, F., et al., Canadian Mineralogist 47 (2009), in press		
GDAGA	STEROPESITE	Tl_3BiCl_6	
SERIES H	HEKLAITE, orth/Pnma. The structure corresponds to the synthetic compound $KNaSiF_6$. Garavelli, A., Balić-Žunić, T., Mitolo, D., Acquafredda, P., Leonardsen, E., Jakobson, S.P. (2010): Heklaite, $KNaSiF_6$, a new fumarolic mineral from Hekla volcano, Iceland. Mineralogical Magazine, 74, 147-157.		
GDAHA	HEKLAITE	$KNaSiF_6$	
TYPE B	HYDROUS HALIDES		
SERIES A	DOUGLASITE, mon/. Structure not known. Ochsenius (1877) Steinsalzlager, Halle: 94.		
	Precht, H. (1880): Ueber die Bildung des Wasserstoffs in den Stassfurter Precht Kalisalzbergwerken.- Berichte der Deutschen Chemischen Gesellschaft Berlin 13, 2326-2328.		
	Boeke (1909) Neues Jahrbuch für Mineralogie, Geologie und Paleontologie, Heidelberg, Stuttgart: II: 44.		
	Larsen, E.S. (1921) The Microscopic Determination of the Nonopaque Minerals, First edition, USGS Bulletin 679: 69.		
	Palache, Charles, Harry Berman & Clifford Frondel (1951), The System of Mineralogy of James Dwight Dana and Edward Salisbury Dana Yale University 1837-1892, Seventh edition, Volume II: 100.		
GDBAA	DOUGLASITE	$K_2FeCl_4 \cdot 2H_2O$	

SERIES B	ERYTHROSIDERITE SERIES, orth/Pnma. Structure consists of $[\text{Fe}^{3+}\text{Cl}_5\text{H}_2\text{O}]^{2-}$ octahedra that are connected by 2K^+ to form a fluorite-like arrangement.	
GDBBA	ERYTHROSIDERITE	$\text{K}_2\text{FeCl}_5\cdot\text{H}_2\text{O}$
GDBBB	KREMERSITE	$(\text{NH}_4,\text{K})_2\text{FeCl}_5\cdot\text{H}_2\text{O}$
GROUP E	CHAIN STRUCTURES	
TYPE A	ANHYDROUS HALIDES	
SERIES A	CALOMEL SERIES, tetr/14/mmm. Structure consists of linear Cl-Hg-Hg-Cl molecules // [001] that are linked into sheets // (001) of alternating Cl and Hg atoms. The structure of moschelite consists of linear dimers I-Hg-Hg-I extending along the c axis with an Hg-Hg distance of 2.5903 Å. The overall coordination sphere of the Hg atom is a considerably distorted octahedron.	
GEAAA	CALOMEL	Hg_2Cl_2
GEAAB	KUZMINITE	$\text{Hg}_2(\text{Br},\text{Cl})_2$
GEAAC	MOSCHELITE	Hg_2I_2
SERIES B	RUTILE Structure type, tetr/P4₂/mnm.	
GEABA	SELLAITE	MgF_2
SERIES C	EGLESTONITE, cub/1a3d. The structure of eglestonite consists of four interpenetrating cubic nets of composition $(\text{Hg}_2)_3\text{O}_2$ in which O atoms form three O-Hg bonds and are connected by Hg-Hg dumbbells situated along each link of the net. The nets are held together by short O-H-O bonds and by Cl ions coordinated to six Hg atoms in the form of a distorted octahedron.	
GEACA	EGLESTONITE	$(\text{Hg}_2)_3\text{Cl}_3\text{O}_2\text{H}$
GEACB	KADYRELITE	$(\text{Hg}_2)_2\text{O}(\text{Br},\text{Cl})_2$
SERIES D	TERLINGUAITE, mon/C2/c, C2/m, C2. The structure consists of a $\text{Hg}^{1+}_3\text{O}_2$ layers interleaved with Hg-O and Hg-Cl layers. The dominating feature of this layer is the Hg^{1+}_3 trimer, in which there is a bonding interaction between adjacent Hg cations. Within the plane, Hg trimers are arranged at the nodes of a 6_3 net, and intertrimer linkage is provided by O atoms. The difference between pinchite and terlinguaite lies in the structure of the Hg-O layers. In terlinguaite, zigzag -Hg-O-Hg-O- chains and Cl-Hg-Hg-Cl molecules, similar to calomel, form pseudo-layers // (101). In kelyanite, the structure consists of Hg atoms that form six crystallographically independent pairs with Hg-Hg distances of 2.48 Å, the Hg and O atoms for O-Hg-Hg-O systems. Hg atoms in the pairs have additional coordination to O, Cl, and Br atoms. Three independent Sb atoms are octahedrally coordinated by O atoms. The Hg dumbbells link the Sb octahedra in a 3D structure. The Sb^{3+}O_6 groups in the structure of kelyanite are not isolated as in other structures with trivalent Sb but participate in a more complex fragment $(\text{Hg}_2)_6\text{O}_6\text{Sb}$ with six Hg-Hg-O-Sb bonds.	
GEADA	TERLINGUAITE	$\text{Hg}^{1+}_2\text{Hg}^{2+}_2\text{O}_2\text{Cl}_2$
GEADB	POYARKOVITE	Hg_3OCl
GEADC	KELIANITE	$(\text{Hg}^{1+})_6(\text{SbO}_6)\text{BrCl}_2$ trig/P3
SERIES E	MENDIPITE, orth/P2₁2₁2₁. In mendipite, Pb is at the apex of a $\text{Pb}(\text{O},\text{Cl})_4$ pyramid; the pyramids share edges to form double chains // [001]; the double chains are linked by sharing Cl atoms. Both structures are based on $[\text{O}_2\text{Pb}_3]$ double chains of edge-sharing OPb_4 ococentered tetrahedra that extend // to the a and b axis in damaraite and mendipite, respectively. In mendipite, the chains occur in two mutually perpendicular orientations, whereas, in damaraite, the chains occur in two orientations inclined to each other by $\sim 50^\circ$. In mendipite, the chains are linked through weak Pb-Cl bonds only, whereas in damaraite, the $[\text{O}_2\text{Pb}_3]$ chains are linked through OH(3) groups to form an $[\text{Pb}_3\text{O}_2](\text{OH})$ sheet that is // to (010). Additional OH(4) groups in damaraite are attached to the $[\text{O}_2\text{Pb}_3]$ double chains. The OH groups in damaraite form two short (OH)-Pb bonds that results in (OH) Pb_2 dimers.	
GEAEA	MENDIPITE	$\text{Pb}_3\text{O}_2\text{Cl}_2$

GEAEB	DAMARAITE	$\text{Pb}_3\text{O}_2(\text{OH})\text{Cl}$ orth/Pmc ₂ ₁
SERIES F	open	
SERIES G	PINCHITE, orth/lbam. The structure consists of layers of HgCl and Hg ₃ O ₄ composition and is closely related to the structure of terlinguaite. There are three distinct Hg positions: Hg1 is coordinated by two O and four Cl atoms in a distorted octahedral arrangement; Hg2 is coordinated by four O and two Cl atoms in a bi-diminished, Siamese dodecahedral arrangement; Hg3 is coordinated by four O atoms in a distorted tetrahedral arrangement.	
GEAGA	PINCHITE	Hg ₅ O ₄ Cl ₂
SERIES H	BRONTESITE, ortho/Pnma. The structure contains one independent eight-coordinated Pb atom located on a .m. symmetry site; the coordination polyhedron is a bicapped trigonal prism with Pb-Cl distances ranging from 2.777 to 3.724 Å. The Pb polyhedra are connected by shared edges to form chains running along [100]. There are also two independent sites occupied by the ammonium ions.	
GEAHA	BRONTESITE	(NH ₄) ₃ PbCl ₅
SERIES I	HANAWALTITE, orth/Pbma. The structure consists of undulatory [Hg-Hg] ²⁺ ribbons which roughly parallel (100). The diatomic [Hg-Hg] ²⁺ groups have anion tails which, in turn, serve as cross linkages between dimer ribbons through [Hg ²⁺ O ₂ Cl ₂] planar rhombs.	
GEAIA	HANAWALTITE	Hg ₆ ¹⁺ Hg ²⁺ [Cl,(OH)] ₂ O ₃
SERIES J	AURIVILLIUSITE, mon/ C2/c. Structure consists of infinite zigzag Hg ²⁺ -O-Hg ²⁺ chains, running in the y direction, condensed by the Hg ⁺ -Hg ⁺ groups to form folded layers which are further connected to form a three-dimensional structure by weak Hg ²⁺ -O bonds.	
GEAJA	AURIVILLIUSITE	[Hg ⁺ Hg ²⁺ O]₂
SERIES K	YEOMANITE, orth/Pnma. The structure is based upon oxocentred OPb ₄ tetrahedra, which jointly with OHPb ₃ triangles, form [O(OH)Pb ₂] ⁺ chains similar to those observed in synthetic Pb ₂ O(OH). Yeomanite is structurally related to sidpietersite, penfieldite and laurionite. Turner, R.W., Siidra, O.I., Rumsey, M.S., Polekhovsky, Y.S., Krivovichev, S.V., Kretser, Y.L. and Stanley, C.J. (2013) Yeomanite, IMA 2013-024. CNMNC Newsletter No. 16, August 2013, page 2706; Mineralogical Magazine, 77, 2695-2709.	
GEAKA	YEOMANITE	Pb ₂ O(OH)Cl
SERIES L	RUMSEYITE, tetr/I4/mmm. The crystal structure consists of alternating [OFPb ₂] and Cl layers. Rumseyite is related to other layered Pb oxyhalides. F and O are statistically disordered over one crystallographic site.	
GEALA	RUMSEYITE	[Pb ₂ OCIF] ₂
TYPE B	HYDROUS HALIDES	
SERIES A	CLARINGBULLITE, hex/P6₃/mmc. The structure contains two Cu positions. The Cu(1) position is octahedrally coordinated by four (OH) groups and two Cl atoms. The Cl(1) atoms are located in the apical position of a (4 + 2)-distorted octahedron, the distortion of which is attributed to the Jahn-Teller effect. The Cu(2) position is coordinated by six (OH) groups in a distorted trigonal prismatic arrangement. The Cu(1)∅ ₆ octahedra share edges to form sheets of octahedra parallel to (001), with every fourth octahedral site vacant. These sheets of octahedra share Cl atoms along [001], and thus creating a framework structure. The stacking of sheets of octahedra is such that the holes in the sheets are collinear, forming channels through the structure parallel to [001]. The Cl(2) position, which is partially occupied by (OH), is located in these channels, at a point midway between the sheets of octahedra. The Cu(2) position is located between the sheets, further linking the [Cu(1) ₃ ∅ ₈] sheets of octahedra into a framework. No structural description for barlowite.	

GEBAA	CLARINGBULLITE	$\text{Cu}_4\text{FCI}(\text{OH})_6$
GEBAB	BARLOWITE	$\text{Cu}_4\text{BrF}(\text{OH})_6$
SERIES B	CONNELLITE SERIES, hex/P6₂c. The structure consists of an intricate three-dimensional framework that contains large channels parallel to the c axis. The framework is composed of edge and corner-sharing polyhedra with Cu^{2+} as the central ion and apices composed of (OH), Cl, and H ₂ O. The polyhedra are distorted. The channel contains the disordered SO_4 ion.	
GEBBA	CONNELLITE	$\text{Cu}_{19}\text{Cl}_4(\text{SO}_4)(\text{OH})_{32}\cdot 3\text{H}_2\text{O}$
GEBBB	BUTTGENBACHITE	$\text{Cu}_{36}\text{Cl}_{6.5}(\text{NO}_3)_{1.5}(\text{OH})_{64}\cdot 5.5\text{H}_2\text{O}$
SERIES C	CHLOROXIPHITE, mon/P2₁/m. PbO_4Cl_4 antiprisms, as in diaboleite, PbO_5Cl_2 polyhedra, and $\text{Cu}(\text{OH})_4\text{Cl}_2$ octahedra, as in diaboleite, but face-sharing to form zigzag chains along [010], build up sheets // (101), which are connected via common Cl ions. New structure data gives a structure containing three symmetrically unique Pb sites and one Cu site. The Cu-site is coordinated by four (OH) groups to form an almost planar $\text{Cu}(\text{OH})_4$ square that is complemented by two apical Cl anions, forming an elongated $[\text{Cu}(\text{OH})_4\text{Cl}_2]$ octahedron. The structure can be described in terms of oxocentred Opb_4 tetrahedra. The OPb_4 tetrahedra link together via common edges to form $[\text{O}_2\text{Pb}_3]^{2+}$ double chains. The difference between chloroxiphite and other natural oxyhalides is the presence of Cu^{2+} cations which form an independent structural unit that links to units formed by OPb_4 tetrahedra. Chloroxiphite can be considered as a modular structure consisting of both strong and anion-centered units.	
GEBCA	CHLOROXIPHITE	$\text{Pb}_3\text{CuO}_2(\text{OH})_2\text{Cl}_2$
SERIES D	YEDLINITE, trig/R3. The structure consists of a coordination framework centered around the Pb atoms. The main irregular polyhedron is formed by Pb coordinated by two X oxygen atoms, one Y oxygen atom, and five Cl atoms. A sixth Cl atom is not included in the coordinating group. Three symmetry-related lead polyhedra share faces, each face consisting of one Cl, one X oxygen and one Y oxygen, to form a planar three membered "pinwheel" centered on a <u>3</u> axis. Each pinwheel shares six Cl-Cl edges with the centro-symmetrically related pinwheel above or below on the <u>3</u> axis. These double pinwheel groups are linked to form stacks parallel to c by octahedrally coordinated Cr atoms (the first case of octahedrally coordinated Cr^{3+} in an oxidized environment). Each lead polyhedron is tied to a symmetry-centered-related polyhedron of an adjacent <u>3</u> axis by sharing an approximately square face composed of four Cl atoms. This face sharing, coupled with additional sharing of edges and apices, serves to unite adjacent stacks to form a three-dimensional bonding framework.	
GEBDA	YEDLINITE	$\text{Pb}_6\text{Cr}^{3+}(\text{O},\text{OH})_8\text{Cl}_6$
SERIES E	CHRYSOTHALLITE, tetr/I4/mmm. The structure consists of the basic structural unit of a (001) layer of edge-sharing distorted $\text{CuCl}_4(\text{OH})_2$ octahedra. Two Ti^{3+} cations occupy the center of isolated TiCl_6 and $\text{TiCl}_4(\text{H}_2\text{O})_2$ octahedra connected to each other and to the Cu polyhedral layers via KCl_6 and KCl_9 polyhedra. Pekov, I.V., Zubkova, N.V., Belakovskiy, D.I., Vigasina, M.F., Sidorov, E.G. and Pushcharovsky, D.Y. (2013) Chrysothallite, IMA 2013-008. CNMNC Newsletter No. 16, August 2013, page 2702; <i>Mineralogical Magazine</i> , 77 , 2695-2709.	
GEBEA	CHRYSOTHALLITE	$\text{K}_6\text{Cu}_6\text{Ti}_3\text{Cl}_{17}(\text{OH})_4\cdot \text{H}_2\text{O}$
SERIES F	ZHARCHIKHITE, mon/P2₁/a. Structure not known. Bolokhontseva S.V., Baturin S.V., Ilmeyer E.S., Papova M.A., Purusova S.P. (1988) Zharchikhite $\text{AlF}(\text{OH})_2$ - a new mineral. Zapiski Vses.Mineral.Obshch., 117, 79-83. American Mineralogist (1989): 74, 504.	
GEBFA	ZHARCHIKHITE	$\text{Al}(\text{F},\text{OH})_3$
GROUP F	LAYERED STRUCTURES	
TYPE A	ANHYDROUS HALIDES	
SERIES A	LAWRENCITE SERIES, trig/R3m. Structure consists of sheets of edge-sharing MCl_6 octahedra, as in brucite, but with 123-123 stacking.	

GFAAA	LAWRENCITE	FeCl ₂	
GFAAB	SCACCHITE	MnCl ₂	
GFAAC	CHLOROMAGNESITE (Q)	MgCl ₂	
SERIES B	TOLBACHITE, mon/C2/m. The structure contains corrugated sheets of distorted Cu²⁺Cl₆ octahedra, with Van der Waals forces providing the intra-sheet bonding.		
GFABA	TOLBACHITE	CuCl ₂	
SERIES C	MOLYSITE, trig/R3. Structure consists of edge-sharing FeCl₃ octahedra forming sheets // (0001) of gibbsite-like interconnected 6-membered rings. The sheets are linked by van der Waals forces, and are stacked in the order ABCABC...		
GFACA	MOLYSITE	FeCl ₃	
SERIES D	FLUORCERITE SERIES, hex/P3c. Structure consists of sheets of F atoms alternating with sheets of REE and F atoms // (0001); the F atoms form 6-membered rings, similar to those in graphite; linear channels // [0001] accommodate additional F atoms.		
GFADA	FLUORCERITE-(Ce)	(Ce,La)F ₃	
GFADB	FLUORCERITE-(La)	(La,Ce)F ₃	
SERIES E	MATLOCKITE SERIES, tetr/P4/nmm. The structure is based on an heterogeneous packing, where the packing atoms are not all alike but of two categories; Cl (larger) and F. All form square layers (Q) which stack in the closest way. The Pb atoms are located between the two layers and are 9-coordinated.		
GFAEA	MATLOCKITE	PbFCl	
GFAEB	ZAVARITSKITE	BiOF	
GFAEC	BISMOCLITE	BiOCl	
GFAED	DAUBREEITE	BiO(OH,Cl)	
GFAEE	RORISITE	CaFCl	
GFAEF	ZHANGPEISHANITE	BaFCl	
SERIES F	BLIXITE, mon/C2/c. Structure is based on oxocentered tetrahedra (OPb₄) that share edges to form [O₅Pb₈] sheets // to (100). Hydroxyl groups form two short (OH)-Pb bonds that result in (OH)Pb₂ dimers attached to the [O₅Pb₈] sheets. Chlorine atoms link the {[O₅Pb₈](OH)₂} sheets in the third dimension. The structure is closely related to other structures based on PbO-type defect sheets.		
GFafa	BLIXITE	Pb ₈ O ₅ (OH) ₂ Cl ₄	
SERIES G	NADORITE, orth/Bmmb. The structure is based on an heterogeneous packing of Cl and O atoms. The square packing layers of Cl and of O atoms alternate and stack in the closest way. The stacking symbol for such a kind of sequence is (Q²Q¹)f. The Pb and Sb atoms occupy 1/2 of the 8-coordinated voids of this packing. Ecdemite and heliophyllite are placed here because they are close members of the bismuth oxy-halide structure and show close structural relations to it.		
GFAGA	NADORITE	PbSbO ₂ Cl	
GFAGB	PERITE	PbBiO ₂ Cl	
GFAGC	THORIKOSITE	Pb ₃ (Sb,As)O ₃ (OH)Cl ₂	tetr/14/mmm
GFAGD	FREEDITE	Pb ₁₅ (Cu,Fe) ₃ ²⁺ As ₄ ³⁺ O ₁₉ Cl ₁₀	mon/C2/m
GFAGE	TELLUOPERITE	Pb ₃ TeO ₄ Cl ₂	
GFAGF	ECDEMITTE	Pb ₆ As ₂ O ₇ Cl ₄ ?	

GFAGG	HELIOPHYLLITE	$Pb_6As_2O_7Cl_4$?
GFAGH	open	
GFAGI	open	
GFAGJ	PINALITE	$Pb_3WO_5Cl_2$
SERIES H	ONORATOITE, tric/P1. The structure consists of SbO_{3+1} trigonal pyramids, with Sb in the center, share edges to form ladder-like double chains // [010]; four of these ladders are linked by shared corners to form tubes // [010]; Cl is accommodated in large cavities between the tube structures.	
GFAHA	ONORATOITE	$Sb_8O_{11}Cl_2$
SERIES I	MELANOTHALLITE, orth/Fddd. Structure not known. Scacchi, A. (1870) Reale accademia delle scienze fisiche e matematiche, Naples, Rend.: 9: 86. Scacchi (1884) Reale accademia delle scienze fisiche e matematiche, Naples, Rend.: 10: 158. Zambonini, Ferruccio (1935) Mineralogia Vesuviana. second edition with Quercigh, 463 pp., Naples: 111-112. Palache, Charles, Harry Berman & Clifford Frondel (1951), The System of Mineralogy of James Dwight Dana and Edward Salisbury Dana Yale University 1837-1892, Volume II: Halides, Nitrates, Borates, Carbonates, Sulfates, Phosphates, Arsenates, Tungstates, Molybdates, Etc. John Wiley and Sons, Inc., New York, 7th edition, revised and enlarged: 44. American Mineralogist (1983): 68: 852. Zapiski Vserossiyskogo Mineralogicheskogo Obshchestva: 111: 562-565.	
GFAIA	MELANOTHALLITE	Cu_2OCl_2
SERIES J	ASISITE, tetr/I4/mmm. Both minerals have sheet structures consisting of two types of layers // (001); in the one layer, PbO_4Cl_4 antiprisms share edges with PbO_4 pyramids; in the other, similar antiprisms also share faces along (001) mirror planes; the positions of Si and Mo are unknown. The new mineral janchevite was discovered in Mn-oxide ore from the Kombat mine, Grootfontein district, Otjozondjupa region, Namibia. Associated minerals are baryte, hausmannite, calcite, magnesite, and kombatite. Janchevite forms orange-red thick tabular anhedral to subhedral grains up to $0.4 \times 0.8 \times 0.8$ mm in size. The luster is adamantine. The mineral is brittle, with Mohs' hardness of $2\frac{1}{2}$. Distinct cleavage on {001} is observed. Dcalc = 8.16 g/cm³. The reflectance values [Rmax/Rmin, % (λ, nm)] are: 20.56/20.06 (470), 19.20/18.81 (546), 19.06/18.59 (589), 19.31/18.85 (650). An infrared spectrum indicates the absence of H-bearing groups and indicates V and Mo valences of 5+ and 6+, respectively. The chemical composition is (electron microprobe, wt.%): PbO 91.64, SiO₂ 0.45, V₂O₅ 1.95, MoO₃ 2.41, Cl 4.16, -O=Cl -0.94, total 99.67. The empirical formula based on (Pb + V + Mo + Si) = 8 apfu is $Pb_7.20V_5+0.38Mo_6+0.29Si_0.13Cl_2.06O_8.25$. Janchevite is the V-dominant analogue of parkinsonite. The mineral is tetragonal and its unit-cell parameters as determined from single-crystal X-ray diffraction data are: a 3.9591(5), c 22.6897(3) Å, V 355.65(1) Å³; Z = 1. Powder X-ray diffraction data conform to the space group I4/mmm; the strongest lines of the PXRD pattern [d, Å (I/I₀, %) (hkl)] are: 3.889 (24) (011), 3.501 (31) (013), 2.979 (86) (015), 2.833 (25) (008), 2.794 (100) (110), 1.992 (26) (118), 1.988 (49) (020), 1.649 (46) (215). Janchevite is named in honor of the prominent Macedonian mineralogist Prof. Dr. Simeon Janchev (b. 1942).	
GFAJA	ASISITE	$Pb_7SiO_8Cl_2$
GFAJB	PARKINSONITE	$(Pb,Mo,\square)_8O_9Cl_2$
GFAJC	SCHWARTZEMBERGITE	$Pb^{2+}_5{}^{3+}O_6H_2Cl_3$
GFAJD	JANCHEVITE	$Pb_7V^{5+}(O_{8.5}\square_{0.5})Cl_2$
SERIES K	PONOMAREVITE, mon/C2/c. Four corner-sharing $CuCl_4$ tetrahedra form Cu_4OCl_{10} clusters; these are linked by K into a 3-dimsional framework	
GFAKA	PONOMAREVITE	$K_4Cu_4OCl_{10}$
SERIES L	open	

SERIES M	SEELIGERITE, orth/Cmm2. Structure consists of a stacking sequence along [001] of square-net layers of O atoms and square-net layers of Cl atoms with Pb ²⁺ and I ⁵⁺ cations located in the voids of the packing. As is typical of cations with a stereoactive lone-pair of electrons, Pb ²⁺ and I ⁵⁺ adopt strongly-asymmetrical configurations. Pb cations occur in a variety of coordination polyhedra, ranging from anticubes and monocapped anticubes to pyramidal 'one-sided' coordinations. I is coordinated by a square of four oxygen atoms.		
GFAMA	SEELIGERITE	Pb ₃ I ₂ O ₄ Cl ₃	
SERIES N	LAURIONITE, orth/Pcmm. In both dimorphs, Pb ^[3+3+2] bicapped trigonal prisms share trigonal faces to form columns // [010]. In paralaurionite, the prisms in the columns share square faces to form double columns; in laurionite, the prisms in the columns share Cl-Cl edges to form zigzag chains // [001], resulting in sheets // (100).		
GFANA	LAURIONITE	Pb(OH)Cl	orth/Pcmm
GFANB	PARALAURIONITE	Pb(OH)Cl	mon/C2/m
SERIES O	FIEDLERITE, mon/P2 ₁ /a. In both dimorphs, three types of bicapped trigonal prisms, bicapped by F + water, Cl + (OH) or Cl+F, share trigonal faces to form columns // [010], and edges to form chains // [001], resulting in sheets // (100).		
GFAOA	FIEDLERITE	Pb ₃ (OH) ₂ Cl ₄	mon/P2 ₁ /a
SERIES P	PENFIELDITE, hex/P6/m. Pb ^[3+3+2] bicapped trigonal prisms share edges and corners to form a hexagonal framework with channels // [0001].		
GFAPA	PENFIELDITE	Pb ₂ (OH)Cl ₃	
SERIES Q	KOENENITE, trig/R3m. Structure consists of two types of sheets // (0001), regularly alternating in the [0001] direction: I. NaCl-type sheets with [111] _{NaCl} perpendicular to (0001), and II. Brucite-type sheets; both types are rotated 28.2 degrees to each other around [0001]. One double sheet (I + II) has c = 10.88Å.		
GFAQA	KOENENITE	Na ₄ Mg ₉ Al ₄ (OH) ₂₂ Cl ₁₂	
SERIES R	TEDHADLEYITE, tric/A1. The crystal structure of tedhadleyite, ideally Hg ₂ +Hg ₁₀ O ₄ I ₂ (Cl,Br) ₂ , triclinic, A-1, a 7.0147(5), b 11.8508(7), c 12.5985(8) Å, alpha 115.583(5), beta 82.575(2), gamma 100.619(2)°, V 927.0(2) Å ³ , Z = 2, was solved by direct methods and refined to an R1 index of 4.5% for 2677 unique reflections. There are six symmetrically distinct Hg sites in tedhadleyite: Hg(1) is occupied by Hg ²⁺ and Hg(2-6) are occupied by Hg ⁺ that forms three [Hg-Hg] ₂ ⁺ dimers with Hg-Hg separations between 2.527 and 2.556 Å. These [Hg-Hg] ₂ ⁺ dimers have strong covalent bonds to O atoms, forming pseudo-linear O-Hg-Hg-O arrangements, and weak bonds to halogen and O atoms at high angles to the dimer axis. The [O-Hg-Hg-O] groups share anions to form four-membered square rings of composition [Hg ₈ O ₄] that link along [100] via [O-Hg-Hg-O] groups and along [001] via [O-Hg-O] groups, forming rectangular rings of composition [Hg ₁₄ O ₈]. The rings form a corrugated layer that interweaves with a symmetrically related layer whereby the [O-Hg(6)-Hg(6)-O] linking groups of one layer pass through the centres of the square [Hg ₈ O ₄] rings of the other layer to form [Hg ₁₁ O ₄] complex slabs parallel to (010) that link through Hg-I and Hg-Br,Cl bonds.		
GFARA	TEDHADLEYITE	Hg ²⁺ (Hg ¹⁺ -Hg ¹⁺) ₅ O ₄ I ₂ (Cl _{1.16} Br _{0.84})	
SERIES S	SYMESITE SERIES, mon/Cm. The crystal structure of mereheadite (monoclinic, Cm, a = 17.372(1), b = 27.9419(19), c = 10.6661(6) Å, β = 93.152(5)°, V = 5169.6(5) Å ³) has been solved by direct methods and refined to R1 = 0.058 for 6279 unique observed reflections. The structure consists of alternating Pb-O/OH blocks and Pb-Cl sheets oriented parallel to the (201) plane and belongs to the 1:1 type of lead oxide halides with PbO blocks. It contains 30 symmetrically independent Pb positions, 28 of which belong to the PbO blocks, whilst two positions (Pb12 and Pb16) are located within the tetragonal sheets of the Cl- anions. Mereheadite is thus the first naturally occurring lead oxychloride mineral with inter-layer Pb ions. The coordination configurations of the Pb atoms of the PbO blocks are distorted versions of the square antiprism. In one half of the coordination hemisphere, they are coordinated by hard O ²⁻ and OH- anions whose number varies from three to four, whereas the other		

coordination hemisphere invariably consists of four soft Cl⁻ anions located at the vertices of a distorted square. The Pb₁₂ and Pb₁₆ atoms in between the PbO blocks have an almost planar square coordination of four Cl⁻ anions. These PbCl₄ squares are complemented by triangular TO₃ groups (T = B, C) so that a sevenfold coordination is achieved. The Pb-O/OH block in mereheadite can be obtained from the ideal PbO block by the following list of procedures: (1) removal of some PbO₄ groups that results in the formation of square-shaped vacancies; (2) insertion of TO₃ groups into these vacancies; (3) removal of some Pb atoms (that correspond to the Pb1A and Pb2A sites), thus transforming coordination of associated O sites from tetrahedral OPb₄ to triangular OHPb₃; and (4) replacement of two O²⁻ anions by one OH⁻ anion with twofold coordination; this results in formation of the 1 x 2 elongated rectangular vacancy. The structural formula that can be derived on the basis of the results of single-crystal structure determination is Pb₄₇O₂₄(OH)₁₃Cl₂₅(BO₃)₂(CO₃). Welch et al. (1998) proposed the formula Pb₂O(OH)Cl for mereheadite, which assumes that neither borate nor carbonate is an essential constituent of mereheadite and their presence in the mineral is due to disordered replacements of Cl⁻ anions. However, our study demonstrates that this is not the case, as BO₃ and CO₃ groups have well-defined structural positions confined in the vacancies of the Pb-O/OH blocks and are therefore essential constituents. Our results also show that mereheadite is not a polymorph of blixite, but is in fact related to symesite. Symesite thus becomes the baseline member of a group of structurally-related minerals. The structure of hereroite contains 16 independent Pb sites in strongly asymmetric coordination by O and Cl atoms. There are two tetrahedral sites, from which one (As) is occupied solely by As, whereas the second (T) has a mixed occupancy of [Si_{0.48}As_{0.29}V_{0.15}Mo_{0.09}]. There are 21 O sites. The O1-O8 sites belong to the AsO₄ and TO₄ tetrahedral oxyanions. The other O atoms are tetrahedrally coordinated by Pb atoms, thus being central for the OPb₄ oxocentered tetrahedral. These tetrahedral share edges to form the [O₂₁Pb₃₂]²²⁺ layers that can be described as derivatives of the [OPb] layer from the structure of tetragonal PbO. The topology of the [O₂₁Pb₃₂]²²⁺ layer is complex and can be described as a combination of modules extracted from the layers of OPb₄ tetrahedra present in the structures of kombatite and symesite. The structure of hereroite belongs to the 2:1 type of layered Pb oxyhalides and consists of alternating PbO-type layers and Cl sheets oriented // to the (010) plane.

GFASA	MEREHEADITE	Pb ₄₇ O ₂₄ (OH) ₁₃ Cl ₂₅ (BO ₃) ₂ (CO ₃)	mon/Cm
GFASB	SYMESITE	Pb ₁₀ (SO ₄)O ₇ Cl ₄ (H ₂ O)	tri/B ₁
GFASC	VLADKRIVOVICHEVITE	[Pb ₃₂ O ₁₈][Pb ₄ Mn ₂ O]Cl ₁₄ (BO ₃) ₈ ·2H ₂ O	orth/Pmnm
GFASD	HEREROITE	[Pb ₃₂ O ₂₀ (O,□)](AsO ₄) ₂ (Si,As,V,Mo)O ₄] ₂ Cl ₁₀	mon/C2/c
XEALA	BRITVINITE	[Pb ₇ (OH) ₃ (BO ₃) ₂ (CO ₃)] [Mg _{4.5} (OH) ₃ (Si ₅ O ₁₄)]	
KCGID	LEUCOSTAURITE	Pb ₂ [B ₅ O ₉]Cl·0.5H ₂ O	
VAIAA	HYALOTEKITE	Pb ₂ Ba ₂ Ca ₂ [B ₂ (Si _{3/2} Be _{1/2})Si ₈ O ₂₈]F	
GFASE	ERIKJONSSONITE	(Pb ₃₂ O ₂₁)[(V,Si,Mo,As)O ₄] ₄ Cl ₉	

SERIES T **MELLIZINKALITE, tric/P1₁.** The structure consists of alternating layers of different ZnCl₄ polyhedra. The Zn(1) cations are located in flat squares which are connected to each other via common Cl-Cl edges to form Zn₂Cl₆ dimers, whereas Zn(2) cations center isolated tetrahedra. Potassium cations occupy sites between the layers of Zn-centered polyhedra.

GFATA	MELLIZINKALITE	K ₃ Zn ₂ Cl ₇
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TYPE B **HYDROUS HALIDES**

SERIES A **SIMONKOLLEITE, trig/R3m.** The structure consists of Zn octahedron sharing four edges with adjacent octahedra to form a dioctahedral sheet similar to that in muscovite and other dioctahedral phyllosilicates. In this sheet, each vacant octahedron is sandwiched between two Zn tetrahedral with their apices pointing away from the sheet. Related minerals with similar structures include cianciullite, gordaite, namuwite, bechererite, chalcophyllite, ramsbeckite, chalcophanite and claringbullite.

GFBA	SIMONKOLLEITE	[Zn ₅ (OH) ₈ Cl ₂](H ₂ O)
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SERIES B **ARAVAIPAITE SERIES, tric/P1₁ or P1 (βPbF₂ structure).** The structure of these minerals consists of (Pb,Ca)F₂ layers parallel to {010}, with Al-(F,OH) octahedra between layers.

GFBA	ARAVAIPAITE	Pb ₃ Al(F,OH) ₉
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GFBBB	CALCIOARAVAIPATE	$\text{PbCa}_2\text{Al}(\text{F},\text{OH})_9$
SERIES C	NEPSKOEITE, orth/Pcmm,Pcm2₁, or Pc2m. Structures not known. Zapiski Vserossiyskogo Mineralogicheskogo Obshchestva (1998): 127(1): 41-46. Zapiski Vserossiyskogo Mineralogicheskogo Obshchestva: 111: 324-329. American Mineralogist (1983): 68: 643. Acta Crystallographica: 6: 40-44.	
GFBCA	NEPSKOEITE	$\text{Mg}_4\text{Cl}(\text{OH})_7 \cdot 6\text{H}_2\text{O}$
GFBCB	KORSHUNOVSKITE	$\text{Mg}_2\text{Cl}(\text{OH})_3 \cdot 4\text{H}_2\text{O}$
SERIES D	CALUMETITE. Structure not known. Williams, S. A. (1963): Anthonyite and calumetite, two new minerals from the Michigan copper district. American Mineralogist: 48: 614-619.	
GFBD A	CALUMETITE	$\text{CaCu}_4(\text{OH})_8\text{Cl}_2 \cdot 3.5\text{H}_2\text{O}$, orth/
GFBD B	ANTHONYITE	$\text{Cu}(\text{OH},\text{Cl})_2 \cdot 3\text{H}_2\text{O}$, mon/
SERIES E	KHAIDARKANITE, mon/C2/m. Structure consists of $\text{AlF}_4(\text{H}_2\text{O})_2$ distorted octahedra sharing edges to form linear chains // [010]; $\text{Al}(\text{OH})_6$ octahedra and $\text{Cu}(\text{OH})_4(\text{H}_2\text{O})_2$ tetragonal dipyramids sharing edges to form a 3-membered columns also // [010]. The chains and columns are linked by H-bonding and by sharing some corners of the polyhedra.	
GFBEA	KHAIDARKANITE	$\text{Cu}_4\text{Al}_3(\text{OH})_{14}\text{F}_3 \cdot 2\text{H}_2\text{O}$
SERIES F	ROMANORLOVITE, tetr/I4/mmm. Pekov, I.V., Zubkova, N.V., Yapaskurt, V.O., Britvin, S.N., Vigasina, M.F., Lykova, I.S., Sidorov, E.G. and Pushcharovsky, D.Y. (2014) Romanorlovite, IMA 2014-011. CNMNC Newsletter No. 20, June 2014, page 557; <i>Mineralogical Magazine</i> , 78 , 549-558.	
GFBF A	ROMANORLOVITE	$\text{K}_8\text{Cu}_6\text{Cl}_{17}(\text{OH})_3$
SERIES G	KALITHALLITE, tetr/I4/mmm.	
GFBG A	KALITHALLITE	$\text{K}_3\text{TlCl}_6 \cdot 2\text{H}_2\text{O}$

Updated 05/20/19