# **CARBONATES**

CLASS J CARBONATES

GROUP A CARBONATES WITHOUT ADDITIONAL ANIONS, WITHOUT WATER.

TYPE A ALKALI CARBONATES

SERIES A ZABUYELITE, mon/C2/c. Structure consists of planar carbonate groups perpendicular to [001] which

are linked by distorted Li tetrahedra. The structure of natrite contains [001] columns formed by facesharing Na octahedral and further 7-fold coordinated Na polyhedra; the columns are connected by

carbonate groups.

JAAAA ZABUYELITE Li<sub>2</sub>CO<sub>3</sub>

JAAAB GREGORYITE (Na,K,Ca)<sub>2</sub>(CO<sub>3</sub>)

JAAAC NATRITE Na<sub>2</sub>CO<sub>3</sub>

SERIES B NAHCOLITE SERIES, mon/P2<sub>1</sub>c. Structure consists of chains // [001] of edge-sharing Na octahedra;

carbonate triangles are linked by H-bonding to form chains // [10 $\underline{1}$ ], and by Na to form sheets // (101), and a 3-dimensional framework. Structure of kalicinite consists of [(HCO<sub>3</sub>)<sub>2</sub>]<sup>2-</sup> dimmers which are connected by K ions. The teschemacherite structure consists of [CO<sub>2</sub>OH] chains // [001] which are

linked into a framework by H bonds from the [NH<sub>4</sub>]<sup>+</sup> groups.

**JAABA NAHCOLITE** NaHCO<sub>3</sub> mon/P2<sub>1</sub>/c **JAABB KALICINITE** KHCO<sub>3</sub> mon/P2<sub>1</sub>/n **JAABC** (NH<sub>4</sub>)HCO<sub>3</sub> orth/Pnaa **TESCHEMACHERITE JAABD** WEGSCHEIDERITE Na<sub>5</sub>(CO<sub>3</sub>)(HCO<sub>3</sub>)<sub>3</sub> tric/P1

## TYPE B ALKALI-EARTH CARBONATES

SERIES A CALCITE SERIES, trig/R3c. The structure is based on the packing of CO<sub>3</sub> groups, having Ca atoms in the voids of this packing with antiprismatic coordination. The CO<sub>3</sub> groups form planar layers, and

in the voids of this packing with antiprismatic coordination. The CO<sub>3</sub> groups form planar layers, and the structure can be imagined as derived from a distorted hexagonal closest packing of the oxygen atoms with C atoms occupying triangular voids, and the Ca atoms with octahedral coordination. The structure also can be described as having sheets of planar carbonate groups and sheets of corner-sharing Ca octahedra alternating along [0001]. Each O and carbonate group connects a Ca atom of

the underlying sheet to a Ca atom of the overlying sheet, forming a 3-dimensional framework.

JABAA CALCITE CaCO<sub>3</sub> **JABAB MAGNESITE** MgCO<sub>3</sub> **JABAC** SIDERITE FeCO<sub>3</sub> **JABAD** RHODOCHROSITE MnCO<sub>3</sub> **JABAE** SPHAEROCOBALTITE CoCO<sub>3</sub> **JABAF SMITHSONITE** ZnCO<sub>3</sub> **JABAG OTAVITE** CdCO<sub>3</sub> **GASPEITE JABAH** (Ni,Mg)CO<sub>3</sub> NAAAA **NITRATINE** Na[NO<sub>3</sub>]

SERIES B DOLOMITE, trig/R3. The structure is an interstitial substitution derivative of calcite. The substitution

of Ca by Mg occurs in alternate layers. The cations are ordered, with sheets of Ca octahedra

alternating with sheets of the other octahedra along the c-axis.

JABBADOLOMITE $CaMg(CO_3)_2$ JABBBANKERITE $CaFe(CO_3)_2$ JABBCKUTNOHORITE $CaMn(CO_3)_2$ JABBDMINRECORDITE $CaZn(CO_3)_2$ 

**SERIES C** ARAGONITE SERIES, orth/Pmcn. The structure is based on the packing of CO<sub>3</sub> groups, with Ca in voids with a strong distorted cubo-octahedral coordination from 6 to 9. Ca is geometrically

distributed in an hexagonal closest packing.

**JABCA ARAGONITE** CaCO<sub>3</sub> WITHERITE **JABCB** BaCO<sub>3</sub> **JABCC STRONTIANITE** SrCO<sub>3</sub> **JABCD CERUSSITE** PbCO<sub>3</sub> NAABA **NITER** KNO<sub>3</sub>

VATERITE, hex/P63/mmc. Structure consists of layers // (0001) of close-packed carbonate groups **SERIES D** 

alternating with layers of Ca atoms; the carbonate planes are perpendicular to (0001).

**JABDA VATERITE** CaCO<sub>3</sub>

HUNTITE, trig/R32. Structure consists of spiral chains // [0001] of edge-sharing MgO6 octahedra **SERIES E** 

which are linked by sharing corners with CaO<sub>6</sub> trigonal prisms and carbonate triangles.

**JABEA HUNTITE** Mg3Ca(CO3)4 **JABEB NORSETHITE** BaMg(CO<sub>3</sub>)<sub>2</sub>

**SERIES F** BARYTOCALCITE, mon/P2<sub>1</sub>/m. Alstonite is a homeotype of aragonite. The paralstonite structrue

consists of Ba and Ca and planar carbonate ions // (0001).

**JABFA** BARYTOCALCITE BaCa(CO<sub>3</sub>)<sub>2</sub>

**JABFB ALSTONITE** BaCa(CO<sub>3</sub>)<sub>2</sub> tric/C1 or C1

**JABFC** open

**JABFD PARALSTONITE** BaCa(CO<sub>3</sub>)<sub>2</sub> trig/P321 **JABFE OLEKMINSKITE** Sr(Sr,Ca,Ba)(CO<sub>3</sub>)<sub>2</sub> trig/P321

**SERIES G** CARBOCERNAITE, orth/Pmc2<sub>1</sub>, mon/Pm. Chakhmouradian, A.R., Cooper, M.A., Reguir, E.P., Moore, M.A. (2017): Carbocernaite from Bear Lodge, Wyoming: Crystal chemistry, paragenesis, and rareearth fractionation on a microscale. American Mineralogist, 102, 1340-1352.

Zoned crystals of carbocernaite occur in hydrothermally reworked burbankite-fluorapatite-bearing calcite carbonatite at Bear Lodge, Wyoming. The mineral is paragenetically associated with pyrite, strontianite, barite, ancylite-(Ce), and late-stage calcite, and is interpreted to have precipitated from sulfate-bearing fluids derived from an external source and enriched in Na, Ca, Sr, Ba, and rare-earth elements (REE) through dissolution of the primary calcite and burbankite. The crystals of carbocernaite show a complex juxtaposition of core-rim, sectoral, and oscillatory zoning patterns arising from significant variations in the content of all major cations, which can be expressed by the empirical formula (Ca0.43-0.91Sr0.40-0.69REE0.18-0.59Na0.18-0.53Ba0-0.08)∑1.96-2.00(CO3)2. Interelement correlations indicate that the examined crystals can be viewed as a solid solution between two hypothetical end-members, CaSr(CO3)2 and NaREE(CO3)2, with the most Na-REE-rich areas in pyramidal (morphologically speaking) growth sectors representing a probable new mineral species. Although the Bear Lodge carbocernaite is consistently enriched in light REE relative to heavy REE and Y (chondrite-normalized La/Er = 500-4200), the pyramidal sectors exhibit a greater degree of fractionation between these two groups of elements relative to their associated prismatic sectors. A sample approaching the solid-solution midline

[(Ca0.57Na0.42)\(\sum\_0.99\)(Sr0.50REE0.47Ba0.01)\(\sum\_0.98\)(CO3)2] was studied by single-crystal X-ray diffraction and shown to have a monoclinic symmetry [space group P11m, a = 6.434(4), b = 7.266(5), c = 5.220(3) Å,  $\gamma$  = 89.979(17)°, Z = 2] as opposed to the orthorhombic symmetry (space group Pb21m) proposed in earlier studies. The symmetry reduction is due to partial cation order in sevenfold-coordinated sites occupied predominantly by Ca and Na. and in tenfold-coordinated sites hosting Sr, REE, and Ba. The ordering also causes splitting of carbonate vibrational modes at 690-740 and 1080-1100 cm-1 in Raman spectra. Using Raman micro-spectroscopy, carbocernaite can be readily distinguished from burbankite- and ancylite-group carbonates characterized by similar energy-dispersive spectra. Structure not known. A. G. Bulakh, V. V. Kondrat'yeva, Ye. N. Baronova

(1961) Carbocernaite, a New Rare-Earth Carbonate, Zapiski Vses. Mineralog. Obshch., v. 90, p. 42-49.

American Mineralogist: 46: 1202.

Rock and Mineral Museum of the Institute of Geology, Ministry of Metallurgical Industry (1979): First discovery of uranothorite and carbocernaite at Bayan Obo. Geology and Prospecting, 15(8), 21 (in

Harris, Donald C. (1972): Carbocernaite, a Canadian occurrence. Canadian Mineralogist 11, 812-818.

**JABGA CARBOCERNAITE** (Ca,Na)(Sr,Ce,Ba)(CO<sub>3</sub>)<sub>2</sub> orth/Pb2m

**SERIES H** 

BENSTONITE. Structurally related to calcite; one carbonate group is  $/\!\!/$  to (0001) and 12 are somewhat inclined to (0001); there are three Ba<sup>[10]</sup>, three Ba<sup>[9]</sup>, six Ca<sup>[7+1]</sup> and one Mg<sup>[6]</sup> in the formula

unit.

**JABHA BENSTONITE** Ba<sub>6</sub>Ca<sub>6</sub>Mg(CO<sub>3</sub>)<sub>13</sub> R3

TYPE C ALKALI AND ALKALI-EARTH CARBONATES

EITELITE SERIES, trig/R3. The structure consists of sheets of [Mg(CO3)2]2- in which Mg is in almost **SERIES A** perfect octahedral coordination between oxygens of 6 different CO<sub>3</sub> groups. Adjacent Mg-centered octahedra do not share oxygens but do share CO<sub>3</sub> groups. Two Na atoms in 6-fold coordination lie

at different levels between successive Mg carbonate sheets, being alternately attached to the sheet

above or the one below.

**JACAA EITELITE**  $Na_2Mg(CO_3)_2$ BÜTSCHLIITE **JACAB**  $K_2Ca(CO_3)_2$ **NYEREREITE JACAC** Na<sub>2</sub>Ca(CO<sub>3</sub>)<sub>2</sub> **JACAD ZEMKORITE** Na<sub>2</sub>Ca(CO<sub>3</sub>)<sub>2</sub>

**SERIES B** FAIRCHILDITE, hex/P6<sub>3</sub>/mmc. Structure similar to that of neverereite; K<sub>2</sub> and Ca are statistically

distributed over the M sites; only one carbonate group is parallel to (0001).

**JACBA FAIRCHILDITE**  $K_2Ca(CO_3)_2$ 

**SERIES C** SHORTITE, orth/Amm2. Structure consists of Na(CO<sub>3</sub>)₂ and Ca₂NaCO<sub>3</sub> layers. Ca has 9-fold

coordination and Na has 6- and 8-fold coordination.

JACCA SHORTITE Na<sub>2</sub>Ca<sub>2</sub>(CO<sub>3</sub>)<sub>3</sub>

**SERIES D** JUANGODOYITE, mon/P2<sub>1</sub>/a. Structure not known. J. Schlüter, D. Pohl: "Juangodoyite, Na2Cu(CO3)2,

a new mineral from the Santa Rosa mine, Atacama desert, Chile", N. Jb. Min. Abh. 182(1):11-14 (2005)

**JACDA JUANGODOYITE** Na<sub>2</sub>Cu(CO<sub>3</sub>)<sub>2</sub>

TYPE D CARBONATES WITH REE ELEMENTS.

**SERIES A** SAHAMALITE-(CE), mon/P2<sub>1</sub>/a. Structure consist of Ce and Mg polyhedra; carbonate groups are

approximately // (100). Chains of [MgO<sub>2</sub>(CO<sub>3</sub>)<sub>2+2</sub>]<sup>6</sup> polyhedra along [001] are connected into a

framework by De atoms.

**JADAA** SAHAMALITE-(Ce) (Mg,Fe)Ce<sub>2</sub>(CO<sub>3</sub>)<sub>4</sub>

**SERIES B** BURBANKITE SERIES, hex/P63mmc. The structure of this group consists of layering on (010)

> composed of four slabs; 2 x [REE<sub>2</sub>Na(CO<sub>3</sub>)<sub>4</sub>] and 2 x [Na<sub>3</sub>(CO<sub>3</sub>)]. In the first type of slab, the carbonate polyhedra are both flat-lying and inclined standing-on-base, whereas in the second type of

slab, the carbonate polyhedra are approximately flat-lying.

**JADBA BURBANKITE** (Na,Ca)<sub>3</sub>(Sr,Ba,Ca)<sub>3</sub>(CO<sub>3</sub>)<sub>5</sub> hex/P6<sub>3</sub>/mmc hex/P6<sub>3</sub>/mc **JADBB KHANNESHITE** (Na,Ca)<sub>3</sub>(Ba,Sr,Ca)<sub>3</sub>(CO<sub>3</sub>)<sub>5</sub> JADBC REMONDITE-(Ce) Na<sub>3</sub>(Ce,La,Ca,Na,Sr)<sub>3</sub>(CO<sub>3</sub>)<sub>5</sub> mon ps. hex/

JADBD PETERSENITE-(Ce) Na<sub>4</sub>(Ce,La,Nd)<sub>2</sub>(CO<sub>3</sub>)<sub>5</sub> mon/P2<sub>1</sub>

JADBE CALCIOBURBANKITE (Na,Ca)<sub>3</sub>(Ca,REE,Sr)<sub>3</sub>(CO<sub>3</sub>)<sub>5</sub> hex/P6<sub>3</sub>mc,P6<sub>2</sub>c, or P6<sub>3</sub>mmc

JADBF REMONDITE-(La) Na $_3$ (La,Ce,Ca) $_3$ (CO $_3$ ) $_5$  mon. P2 $_1$  JADBG SANROMANITE Na $_2$ CaPb $_3$ (CO $_3$ ) $_5$  hex/P6 $_3$ /mc

GROUP B CARBONATES WITH ADDITIONAL ANIONS, WITHOUT WATER

TYPE A CARBONATES WITH Cu, Co, Ni, Zn, Mg, Mn

SERIES A AZURITE, mon/P2<sub>1</sub>/c. The structure is based on the packing of CO<sub>3</sub> and OH ions with two types of

Cu atoms in the voids of this packing: one with nearly square coordination and the other Cu with

tetragonal pyramidal coordination.

JBAAA AZURITE Cu<sub>3</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>2</sub>

SERIES B MALACHITE SERIES, mon or tric/P2<sub>1</sub>/m, P2<sub>1</sub>/a, P2<sub>1</sub>, P1 or P1. The structure is based on a complex

packing of CO<sub>3</sub> and OH ions, with copper atoms in octahedral voids. The packing can be imagined formed by strong distortion of puckered simple hexagonal layers with the packing atoms are at two different levels. The structures of pokrovskite and glaukosphaerite have been solved. Their structures are built up by ribbons of edge-sharing octahedra running along the c-axis; the ribbons are linked together through corner-sharing giving rise to corrugated layers // to (100) that are interconnected through carbonate groups. The same layers and carbonate groups, arranged in a different orientation with respect to the symmetry operators, built up the structure of malachite.

JBABA ROSASITE CuZnCO<sub>3</sub>(OH)<sub>2</sub>

JBABB POKROVSKITE Mg<sub>2</sub>CO<sub>3</sub>(OH)<sub>2</sub> 0.5H<sub>2</sub>O

**JBABC GLAUKOSPHAERITE** CuNiCO<sub>3</sub>(OH)<sub>2</sub> **JBABD KOLWEZITE** CuCoCO<sub>3</sub>(OH)<sub>2</sub> **JBABE** ZINCROSASITE  $(Zn,Cu)_2CO_3(OH)_2$ **JBABF** MCGUINNESSITE MgCuCO<sub>3</sub>(OH)<sub>2</sub> **JBABG NULLAGINITE** Ni<sub>2</sub>CO<sub>3</sub>(OH)<sub>2</sub> **JBABH MALACHITE** Cu<sub>2</sub>CO<sub>3</sub>(OH)<sub>2</sub> **JBABI GEORGEITE** Cu<sub>2</sub>CO<sub>3</sub>(OH)<sub>2</sub> CHUKANOVITE **JBABJ**  $Fe_2(CO_3)(OH)_2$ **JBABK PARADSASVARITE**  $Zn_2(CO_3)(OH)_2$ 

SERIES C HYDROZINCITE, mon/C2/m. The structure is formed by the packing of CO<sub>3</sub> and OH ions. The Zn

atoms have octahedral and tetrahedral coordination. There are layers of O and OH which contain the Zn atoms in octahedral coordination, with some holes. The Zn atoms occur above and below the holes in the octahedral layers. The complex layers are held together by CO<sub>3</sub> groups situated normal

to the layers.

JBACA HYDROZINCITE  $Zn_5(CO_3)_2(OH)_6$ 

JBACB BRIANYOUNGITE Zn<sub>3</sub>(CO<sub>3</sub>,SO<sub>4</sub>)(OH)<sub>4</sub> orth/B22<sub>1</sub>2

JBACC AURICHALCITE (Zn,Cu)₅(CO₃)₂(OH)<sub>6</sub>

SERIES D HOLDAWAYITE, mon/C2/m. The structure consists of carbonate groups which are linked to five

Mn(O,OH)<sub>6</sub> octahedra in planar units, which in turn are linked parallel to b to form five-octahedronsided tubes extended parallel to b, each having a central ribbing of CO<sub>3</sub> groups. Such columns are cross-linked parallel to c to give slabs parallel to the b-c plane. These in turn are cross-linked so that vacant columns occur between slabs. Each column is a channel defined by superimposed eight-membered rings of edge-sharing Mn(O,OH)<sub>6</sub> octahedra. CI atoms occupy sites along the central axis of these channels and are coordinated only to OH ions through weak H bonds.

JBADA HOLDAWAYITE Mn<sub>6</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>7</sub>(CI,OH)

JBADB DEFERNITE Ca<sub>6</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>7</sub>(OH) nH<sub>2</sub>O orth/Pna2<sub>1</sub> or Pnam

SERIES E LOSEYITE, mon/A2/a. The structure consists of stepped sheets of octahedra oriented parallel to

(001) and connected to each other by isolated tetrahedral and carbonate groups. In loseyite, all the

Zn is tetrahedrally coordinated, and Mg fills in for any deficiency in Zn occupancy.

JBAEA LOSEYITE (Mn,Zn)<sub>7</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>10</sub>

JBAEB SCLARITE (Zn,Mg,Mn)<sub>4</sub>Zn<sub>3</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>10</sub>

TYPE B CARBONATES WITH ALKALIES AND OTHER IONS.

SERIES A DAWSONITE, orth/Imam. Structure consists of edge-sharing AIO<sub>2</sub>(OH)<sub>4</sub> octahedra forming chains

along [001], and edge-sharing  $NaO_4(OH)_2$  pseudo-octahedra forming chains along [100]; carbonate group lie in the (100) plane. In barentsite  $Na(O,F)_6$  and  $AIF_4O_2$  octahedra share edges to form brucite-like sheets // (001); these sheets alternate with layers composed of columns of edge-sharing Na octahedra joined by carbonate groups. The resulting slabs are linked by sharing corners of

octahedra and carbonate groups.

JBBAA DAWSONITE NaAICO<sub>3</sub>(OH)<sub>2</sub>

JBBAB BARENTSITE Na<sub>7</sub>Al(CO<sub>3</sub>)<sub>2</sub>(HCO<sub>3</sub>)<sub>2</sub>F<sub>2</sub>

SERIES B TUNISITE, tetr/P4/nmm. The structure is based on sheets of edge- and corner-sharing OH)<sub>4</sub>O<sub>2</sub>

octahedra // (001), strengthened by carbonate groups. Other features include Na pyramids and Ca

polyhedra.

JBBBA TUNISITE NaCa<sub>2</sub>Al<sub>4</sub>(CO<sub>3</sub>)<sub>4</sub>(OH)<sub>8</sub>Cl

SERIES C SABINAITE, mon/C2/c. The crystal structure is strongly layered and is dominated by a slab

composed of ZrO<sub>8</sub> and TiO<sub>6</sub> polyhedra. The ZrO<sub>8</sub> polyhedra form infinite zig-zag chains along [100]. These chains are cross-linked along [010] by sharing polyhedra edges with like polyhedra in adjacent chains and by sharing edges and corners with TiO<sub>6</sub> octahedra that occupy gaps between the chains. The chains of ZrO<sub>8</sub> polyhedra strongly influence the observed morphology and optical properties of sabinaite. Two distinct carbonate groups are present, one acting as a bidentate ligand in the ZrO<sub>8</sub> polyhedra and the other linking vertices between ZrO<sub>8</sub> and TiO<sub>6</sub> polyhedra. The remaining oxygen atoms from these carbonate groups are shared with the NaO<sub>6</sub> and NaO<sub>8</sub> polyhedra and link the Zr-Ti-O slabs together along [001]. CM-96/811. The structure can also be described as edge-sharing ZrO<sub>8</sub> polyhedra forming zigzag chains // {100} that are cross-linked to adjoining chains

by sharing edges with polyhedra in adjacent chains, and TiO<sub>6</sub> octahedra and carbonate groups between the chains; this creates slabs // (010); the slabs are linked by NaO<sub>8</sub> and NaO<sub>6</sub> polyhedra.

JBBCA SABINAITE Na<sub>4</sub>Zr<sub>2</sub>TiO<sub>4</sub>(CO<sub>3</sub>)<sub>4</sub>

SERIES D ABELLAITE, trig/P63mc. The structure has a known synthetic analogue.

JBBDA ABELLAITE NaPb<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)

TYPE C CARBONATES WITH ALKALI-EARTH CATIONS.

SERIES A BRENKITE, orth/Pbcn. Structure consists of four [FC4] tetrahedra sharing corners to form 4-

membered rings that are linked // [001] by edges and corners; channels // [001] contain Ca ions. In rouvilleite, chains of edge-sharing Ca octahedra // [001] are linked into a framework by (Mn,Ca) octahedra and carbonate groups; Na octahedra and Na hemioctahedra are accommodated in the

cavities.

JBCAA BRENKITE Ca<sub>2</sub>CO<sub>3</sub>F<sub>2</sub>

JBCAB ROUVILLEITE Na<sub>3</sub>(Ca,Mn,Fe)<sub>2</sub>(CO<sub>3</sub>)<sub>3</sub>F

TYPE D CARBONATES WITH REE.

SERIES A CORDYLITE SERIES, hex/P6 $_3$ /mmc. In cordylite, BaO $_{12}$  polyhedra share edges with six adjoining BaO $_{12}$  polyhedra to form sheets // (0001), with six CeO $_9$ F polyhedra in sheets above and below the

BaO<sub>12</sub> polyhedra to form sheets *ii* (600 f), with six CeO<sub>3</sub>F polyhedra in sheets above and below the BaO<sub>1</sub> sheets, and with six CO<sub>3</sub> triangles connecting the sheets; the BeO<sub>9</sub>F polyhedra share three

edges with  $BaO_{12}$  polyhedra, three edges with  $NaO_6$  trigonal prisms, and three edges with  $CO_3$  triangles.

JBDAA CORDYLITE-(Ce) NaBa(Ce,La)<sub>2</sub>(CO<sub>3</sub>)<sub>4</sub>F

JBDAB LUKECHANGITE-(Ce) Na<sub>3</sub>Ce<sub>2</sub>(CO<sub>3</sub>)<sub>4</sub>F

JBDAC CORDYLITE-(La) NaBa(La,Ce)<sub>2</sub>(CO<sub>3</sub>)<sub>4</sub>F

SERIES B KUKHARENKOITE SERIES, mon/P2<sub>1</sub>/m. Structure consists of corner-sharing CeO<sub>9</sub>F polyhedra forming chains // [010]; edge-sharing BaO<sub>7</sub>F<sub>3</sub> and BaO<sub>11</sub> polyhedra form sheets // (010).

JBDBA KUKHARENKOITE-(Ce) Ba<sub>2</sub>Ce(CO<sub>3</sub>)<sub>3</sub>F

JBDBB KUKHARENKOITE-(La) Ba<sub>2</sub>(La,Th,Ce)(CO<sub>3</sub>)<sub>3</sub>F

JBDBC ZHONGHUACERITE-(Ce) Ba<sub>2</sub>Ce(CO<sub>3</sub>)<sub>3</sub>F trig/

SERIES C CEBAITE, mon/Cm/2. Structure consists of double chains of corner-sharing CeO<sub>9</sub>F polyhedra and chains of edge- and corner-sharing Ba polyhedra extending // (010); the chains of CeO<sub>9</sub>F polyhedra are linked by CO<sub>3</sub> ions, and the chains of Ba polyhedra link edges to form Ba<sub>3</sub>O<sub>16</sub> and Ba<sub>3</sub>O<sub>14</sub> blocks.

JBDCA CEBAITE-(Ce) Ba<sub>3</sub>Ce<sub>2</sub>(CO<sub>3</sub>)<sub>5</sub>F<sub>2</sub>

SERIES D SYNCHYSITE SERIES, mon/C2/c. The structure is based on layers of Ca and CeF separated by layers of carbonate groups. The layers stack in a manner analogous to C2/c muscovite, where Ca layers in synchysite are equivalent to K layers in muscovite, CO<sub>3</sub> layers in synchysite, to layers of tetrahedra in muscovite, and CeF layers in synchysite to layers of octahedra in muscovite. Based on the bastnasite layer configuration of (CeF):(CO<sub>3</sub>):[Ca(CO<sub>3</sub>)] 1:1:0 (x2), synchysite has a ratio of 1:1:1 (x6).

JBDDASYNCHYSITE-(Ce) $Ca(Ce,La)(CO_3)_2F$ JBDDBSYNCHYSITE-(Nd) $Ca(Nd,La)(CO_3)_2F$ JBDDCSYNCHYSITE-(Y) $Ca(Y,Ce)(CO_3)_2F$ JBDDDQAQARSSUKITE-(Ce) $BaCe(CO_3)_2F$ 

SERIES E HUANGHOITE-(CE), trig/R3m. CeO<sub>9</sub>F polyhedra share corners to form sheets // (0001); these sheets alternate with sheets of BaO<sub>12</sub> hexagonal prisms and BaO<sub>6</sub>F<sub>6</sub> cubooctahedra; the sheets are linked by carbonate ions.

JBDEA HUANGHOITE-(Ce) BaCe(CO<sub>3</sub>)<sub>2</sub>F trig/

SERIES F PARISITE SERIES, trig/R3 Structure based on the bastnasite structure with additional layers. Based on the bastnasite layer configuration of (CeF):(CO<sub>3</sub>):[Ca(CO<sub>3</sub>)] 1:1:0 (x2), parisite has a ratio of 2:2:1 (x6).

JBDFA PARISITE-(Ce)  $Ca(Ce,La)_2(CO_3)_3F_2$  JBDFB PARISITE-(La)  $Ca(La,Ce)_2(CO_3)_3F_2$ 

JBDFC RONTGENITE-(Ce)  $Ca_2(Ce,La)_3(CO_3)_5F_3$  trig/R3

SERIES G BASTNAESITE SERIES, hex/P $\underline{6}$ 2c. The structure is composed of (0001) layers of Ce and F interspersed with carbonate layers in a 1:1 ratio. The Ce atom is coordinated in CeO $_6$ F $_3$  polyhedra; the three Ce-F bonds are within the (CeF) layer, and that layer is linked to the (CO $_3$ ) layer by interlayer bonding of the Ce atom to six O atoms of the carbonate groups.

JBDGA BASTNAESITE-(Ce) (Ce,La)CO $_3$ F JBDGB BASTNAESITE-(La) (La,Ce)CO $_3$ F JBDGC BASTNAESITE-(Y) (Y,Ce)CO $_3$ F JBDGG THORBASTNAESITE Th(Ca,Ce)(CO<sub>3</sub>)<sub>2</sub> $F_2$ '3H<sub>2</sub>O hex/P $\underline{6}$ 2c

JBDGJ BASTNAESITE-(Nd) NdCO₃F

SERIES H HORVÁTHITE, orth/Pmcn. Structure consist of Na[F3O4] and Y{F4O4] polyhedra which are linked by carbonate groups to form layers // (100); the carbonate groups are also // (100)/CM97-743

JBDHA HORVÁTHITE-(Y) NaY(CO<sub>3</sub>)F<sub>2</sub>

**SERIES I PARATOOITE-(LA), orth/. Structure consists of.** Pring, A., Wallwork, K., Brugger, J., Kolitsch, U. (2006): "Paratooite-(La), a new lanthanum-dominant rare-earth copper carbonate from Paratoo, South Australia",

Mineralogical Magazine 70, 131-138

JBDIA PARATOOITE-(La) (REE,Ca,Na,Sr)<sub>12</sub>Cu(CO<sub>3</sub>)<sub>16</sub>

SERIES J ARISITE SERIES, hex/P6m2. The structure is a member of the flat-lying layered REE fluorcarbonate

group that includes lukechangeite-(Ce), cordylite-(Ce), huanghoite-(Ce), cebaite-

(Ce)mkukharenkoite-(Ce), and kukharenkoite-(La). All of these fluorcarbonates have crystal structures characterized by separate layers of carbonate, F, REE and alkalior alkaline-earth

elements.

Piilonen, P.C., McDonald, A.M., Grice, J.D., Rowe, R., Gault, R.A., Poirier, G., Cooper, M.A., Kolitsch, U., Roberts, A.C., Lechner, W. and Palfi, A.G. (2010): Arisite-(Ce), a new rare-earth fluorcarbonate from the Aris phonolite (Namibia), Mont Saint-Hilaire and the Saint-Amable sill (Québec). Canadian Mineralogist 48, 661-

Structure related to lukechangite-(Ce), cordylite-(Ce), huanghoite-(Ce), horváthite-(Y).

JBDJA ARISITE-(Ce) NaCe<sub>2</sub>(CO<sub>3</sub>)<sub>3</sub>F JBDJB ARISITE-(La) NaLa<sub>2</sub>(CO<sub>3</sub>)<sub>3</sub>F

SERIES K LECOQITE-(Y), hex/P6<sub>3</sub>. Structure consists of the REE atoms surrounded by six O atoms of CO<sub>3</sub>

groups and three water molecules to form a tricapped triangular prism. The Na atoms are centered

in distorted octahedra  $[NaO_4(H_2O)_2]$ , which link to form infinite corrugated chains along c.

JBDKA LECOQITE-(Y) Na<sub>3</sub>Y(CO<sub>3</sub>)<sub>3</sub>.6H<sub>2</sub>O

SERIES L LUSERNAITE-(Y), orth/Pmna. The structure is built by layers // to (010), formed by chains of edgesharing Y-centered polyhedra 9Y1), which run along [100], and are connected along c through Al-

centered octahedra. These chains are decorated on one side by corner-sharing chains of Y-centered polyhedra (Y2), and on the other side by carbonate groups. Along [001] the decorated chains alternate their polarity. Biagioni, C., Bonaccorsi, E., Cámara, F., Cadoni, M., Ciriotti, M.E., Bersani, D., Kolitsch, U. (2012) Lusernaite-(Y), IMA 2011-108. CNMNC Newsletter No. 13, June 2012, page 811; Mineralogical

Magazine, 76, 807-817.

C. Biagioni, E. Bonaccorsi, F. Cámara, M. Cadoni, M. E. Ciriotti, D. Bersani and U. Kolitsch (2012): Lusernaite-(Y), Y4Al(CO3)2(OH)10F·6H2O, a new mineral from Piedmont, Italy. M&M7, 7th Intern. Conf. on Mineralogy & Museums, Dresden, Germany, August 27 - 29, 2012; Program and Abstracts Volume, 85-86. Structure in AM 98(7),

1322, 2013.

JBDLA LUSERNAITE-(Y)  $Y_4AI(CO_3)_2(OH)_{10}F.6H_2O$ 

TYPE E CARBONATES WITH HEAVY METALS.

SERIES A SHANNONITE, orth/P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>. Structure consists of two symmetrically distinct Pb<sup>2+</sup> cations in irregular coordination polyhedra due to the effect of stereoactive s<sup>2</sup> lone-electron pairs. The structure can be described as composed of chains of [OPb<sub>2</sub>] composition running // to [100] that are

built by corner-sharing of [OPb<sub>2</sub>] oxocentred triangles. The [OPb<sub>2</sub>] chains are surrounded by

carbonate groups to form complex [OPb<sub>2</sub>](CO<sub>3</sub>) chains that are linked into a 3-dimensional framework by additional Pb-O bonds. The structure has channels that are // to [100] in which the lone-electron pairs of Pb cations are probably located. Roberts, A. C., Stirling, J. A. R., Carpenter, G. J. C., Criddle, A. J., Jones, G. C., Birkett, T. C. & Birch, W. D. (1995): "Shannonite, Pb2OCO3, a new mineral from the Grand Reef mine, Graham County, Arizona, USA", Mineralogical Magazine: 59: 305-310.

JBEAA SHANNONITE Pb<sub>2</sub>OCO<sub>3</sub>

SERIES B HYDROCERUSSITE, trigonal, P31. Structure consists of layers of carbonate groups // (0001) enclosing a layer of PbO<sub>6</sub>(OH)<sub>4</sub> polyhedra that share corners with the carbonate groups.

JBEBA HYDROCERUSSITE  $Pb_3(CO_3)_2(OH)_2$ JBEBB PLUMBONACRITE  $Pb_5(CO_3)_3O(OH)_2$ 

JBEBC GROOTFONTEINITE Pb<sub>3</sub>O(CO<sub>3</sub>)<sub>2</sub> hex/P6<sub>3</sub>mc

SERIES C PHOSGENITE, tetr/P4/mbm. Structure consists of PbO₄Cl₅ polyhedra that are linked by Cl to form double layers along (001); these are connected by carbonate groups aligned // [001].

JBECA PHOSGENITE Pb<sub>2</sub>(CO<sub>3</sub>)Cl<sub>2</sub>

SERIES D BISM

BISMUTITE SERIES, tetr/I4/mmm. The minerals of this group have double sheets // (001) of edge-sharing BiO $_4$  square pyramids, with stereoactive Bi at the apex, as in litharge; the sheets are connected by O of four CO $_3$  triangles, making the pyramids into square BiO $_{4+4}$  antiprisms. In bismutite there is only this type of double sheet; in kettnerite, this type alternates with a double sheet consisting of a CaF $_4$ O $_4$  square antiprisms and in beyerite it alternates with a single sheet of CaF $_8$  cubes. Structure of kettnerite consists of layers // to (001): the Bi-O layers at z = 0, Ca-F =  $^{1}/_2$ . Both of these layers are pseudotetragonal; showing a subcell. The layers of carbonate groups are located between the BiO and Ca-F layers. The CO $_3$  groups are about // to (110) planes with one O atom oriented towards the Bi-O layer while the remaining two O atoms are oriented towards the Ca-F layer.

JBEDA BEYERITE (Ca,Pb)(BiO)<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>

JBEDB BISMUTITE (BiO)<sub>2</sub>(CO<sub>3</sub>)O<sub>2</sub>

JBEDC KETTNERITE Ca(BiO)CO₃F orth/Pbaa

**SERIES E** 

SOMERSETITE, trig/P31<sub>c</sub>. The new mineral somersetite, has been found at Torr Works ('Merehead quarry') in Somerset, England, United Kingdom. Somersetite is green or white (typically it is similar visually to hydrocerussite-like minerals but with a mint-green tint), forms plates and subhedral grains up to 5 mm across and up to 2 mm thick. In bi-coloured crystals it forms very thin intergrowths with plumbonacrite. The empirical formula of somersetite is Pb8.00C5.00H4.00O20. The simplified formula is Pb8O(OH)4(CO3)5, which requires: PbO = 87.46, CO2 = 10.78, H2O = 1.76, total 100.00 wt.%.

The infrared spectrum of somersetite is similar to that of plumbonacrite and, to a lesser degree, hydrocerussite. Somersetite is hexagonal, P63/mmc, a = 5.2427(7), c = 40.624(6) Å, V = 967.0(3) Å3 and Z = 2. The eight strongest reflections of the powder X-ray diffraction (XRD) pattern [d,Å(I)(hkI)] are: 4.308(33)(103), 4.148(25)(104), 3.581(40)(107), 3.390(100)(108), 3.206(55)(109), 2.625(78)(110), 2.544(98)(0.0.16) and 2.119(27)(1.0.17). The crystal structure was solved from single-crystal XRD data giving R1 = 0.031. The structure of somersetite is unique and consists of the alternation of the electroneutral plumbonacrite-type [Pb5O(OH)2(CO3)3]0 and hydrocerussite-type [Pb3(OH)2(CO3)2]0 blocks separated by stereochemically active lone electron pairs on Pb2+. There are two blocks of each type per unit cell in the structure, which corresponds to the formula of the structure.

[Pb5O(OH)2(CO3)3][Pb3(OH)2(CO3)2] or Pb8O(OH)4(CO3)5 in a simplified representation. The 2D blocks are held together by weak Pb-O bonds and weak interactions between lone pairs.

JBEEA SOMERSETITE Pb<sub>8</sub>O<sub>2</sub>(OH)<sub>2</sub>(CO<sub>3</sub>)<sub>5</sub>

TYPE F CARBONATES WITH HALIDES, SULFATES, PHOSPHATES.

SERIES A NORTHUPITE SERIES, cub/Fd3. Structure consists of NaO<sub>4</sub>Cl<sub>2</sub> distorted octahedra, MgO<sub>6</sub> octahedra and carbonate triangles sharing edges to form a framework. In ferrotychite, clusters of six Na distorted octahedra sharing edges with S tetrahedra are linked by carbonate triangles sharing corners with the Na octahedra; the clusters are connected into a framework by FeO<sub>6</sub> octahedra sharing edges with the carbonate triangles. Structure consists of NaO<sub>4</sub>Cl<sub>2</sub> distorted octahedra, Mg octahedra and carbonate triangles sharing edges to form a framework.

JBFAANORTHUPITE $Na_3Mg(CO_3)_2CI$ JBFABTYCHITE $Na_6Mg_2(CO_3)_4(SO_4)$ JBFACFERROTYCHITE $Na_6Fe_2(CO_3)_4(SO_4)$ 

JBFAD MANGANOTYCHITE Na<sub>6</sub>(Mn,Fe,Mg)<sub>2</sub>(CO<sub>3</sub>)<sub>4</sub>(SO<sub>4</sub>)

BRADLEYITE SERIES, mon/P2<sub>1</sub>/m or P2<sub>1</sub>. Structure consists of corner-sharing MnO<sub>6</sub> octahedra and P tetrahedra forming corrugated sheets // (100); carbonate triangles share edges with the octahedra to form sheets of carbonate groups, also // (100). The Na atoms are accommodated in the corrugations of the octahedral-tetrahedral sheets. In crawfordite, chains of edge-sharing Na octahedra // [001] are connected into sheets // (001) by sharing edges with Na tetrahedra; chains of face-sharing Na octahedra // [001] are linked by P and C groups to form a second kind of sheet; Mn octahedra share edges with CO<sub>3</sub> groups, and corners with P groups; Sr polyhedra share corners to form chains // [010].

JBFBA SIDORENKITE Na<sub>3</sub>Mn(CO<sub>3</sub>)(PO<sub>4</sub>)

JBFBB BONSHTEDTITE Na<sub>3</sub>(Fe,Mg,Mn)(CO<sub>3</sub>)(PO<sub>4</sub>)

JBFBC BRADLEYITE  $Na_3Mg(CO_3)(PO_4)$ JBFBD CRAWFORDITE  $Na_3Sr(CO_3)(PO_4)$ 

SERIES C DAQINGSHANITE SERIES, trigonal/R3m. Structure consists of layers of carbonate triangles and P tetrahedra // (0001) alternating with layers containing Sr and Ce polyhedra; the layers are linked by shared O atoms.

JBFCA DAQINGSHANITE-(Ce)  $(Sr,Ca,Ba)_3(Ce,La)(PO_4)(CO_3)_{3-x}(OH,F)_x$  R32

KABBA NORDENSKIOLDINE CaSn(BO<sub>3</sub>)<sub>2</sub>
KABBB TUSIONITE MnSn(BO<sub>3</sub>)<sub>2</sub>

SERIES D

REEDERITE, hex/P6. The structure contains two different carbonate-containing sheets // (0001), all with the carbonate groups oriented \( \pm \) (0001); one sheet accommodates Na and CI atoms, and the other contains Y and Na atoms; these two sheets form a double layer that alternates with a layer of SO<sub>3</sub>F pyramids and Na atoms .The structure consists of carbonate layers in thick slabs accommodating (CO<sub>3</sub>)<sup>2-</sup> groups oriented perpendicular to the {001} layering, the large cation polyhedra, and the CI ion and (SO<sub>3</sub>F) anions. The Na atoms adopt a variety of distinct coordinations.

JBFDA REEDERITE-(Y) (Na,Mn,Fe)<sub>15</sub>(Y,REE)<sub>2</sub>(CO<sub>3</sub>)<sub>9</sub>(SO<sub>3</sub>F)Cl

SERIES E MINEEVITE, hex/P6<sub>3</sub>/m. The structure contains two different carbonate-containing sheets // (0001), all with the carbonate groups oriented perpendicular (0001); one sheet accommodates Na and CI atoms, and the other contains Y and Na atoms; these two sheets forma double layer that alternates with a layer of SO<sub>3</sub>F pyramids and Na atoms.

JBFEA MINEEVITE-(Y) Na<sub>25</sub>Ba(Y,Gd,Dy)<sub>2</sub>(CO<sub>3</sub>)<sub>11</sub>(HCO<sub>3</sub>)<sub>4</sub>(SO<sub>4</sub>)<sub>2</sub>F<sub>2</sub>Cl

SERIES F PHILOLITHITE, tetr, P4<sub>2</sub>/nnm. Structure consists of chains // [110] and [1<u>1</u>0] of edge-sharing (Mn,Mg)O<sub>6</sub> octahedra are linked by sharing free corners with MnO<sub>4</sub> and SO<sub>4</sub> tetrahedra and carbonate triangles to form an open trellis-like framework with Pb and Cl atoms in the cavities

JBFFA PHILOLITHITE  $Pb_{12}(Mg,Mn)_2(Mn,Mg)_4Mn[Cl_4/O_6/(OH)_{12}/(CO_3)_4/SO_4]$ 

#### **SERIES G**

LEADHILLITE SERIES. Mon/P2<sub>1</sub>/a. Structure consists of three layers: A – S tetrahedra, B – Pb polyhedra and OH ions, and C – Pb polyhedra and carbonate groups; these layers are arranged in the sequence BABCCBABCC... the layers are // (001). The structure of macphersonite has many features in common with its polymorph leadhillite including three distinct types of layers. Layer A includes sulphate tetrahedra, layer B is composed of Pb and OH, which layer C is composed of Pb and CO<sub>3</sub> with topology identical to that in cerussite. In both macphersonite and leadhillite, these layers are stacked along (010) as ...BABCCBABCC... The double CC layer is almost identical in the two structures and forms a structural backbone and occurs in other structures including hydrocerussite and plumbonacrite. The sulfate layer shows the greatest difference between the two structures and can be described by a pattern of up or down pointing tetrahedra. For macphersonite, the sequence along (001) is...UDUDUD... while in leadhillite the sequence along (010) is ...UDUDUDDU... This latter sequence effectively doubles b relative to the equivalent direction in macphersonite. Susannite, a third polymorph, may have yet another sequence of sulfates to give trigonal symmetry.

JBFGALEADHILLITE $Pb_4(CO_3)_2(SO_4)(OH)_2$  $mon/P2_1/a$ JBFGBSUSANNITE $Pb_4(CO_3)_2(SO_4)(OH)_2$ trig/R3JBFGCMACPHERSONITE $Pb_4(CO_3)_2(SO_4)(OH)_2$ orth/Pcab

#### **SERIES H**

PODLESNOITE, orth/Cmcm. Structure consists of columns of Ca-centered 8-fold polyhedra ( $CaO_6F_2$ ) stretched along [001]. Carbonate groups, coplanar to the cs plane, and large Ba atoms are located in cavities of the framework. Ba atoms center the 10-fold polyhedra ( $BaO_6F_4$ ); F atoms center the tetrahedra ( $FCa_2Ba_2$ ). The structure is remotely related to that of minerals of the aragonite group, and can be regarded as a derivative of the aragonite-type structure.

JBFHA PODLESNOITE BaCa<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>F<sub>2</sub>

GROUP C CARBONATES WITHOUT ADDITIONAL ANIONS, BUT WITH WATER.

TYPE A CARBONATES WITH MEDIUM-SIZED CATIONS.

SERIES A LANSFORDITE SERIES, mon/P2<sub>1</sub>/m. Structure consists of edge-sharing MgO<sub>6</sub> octahedra and carbonate groups forming chains // [010]; the chains are linked by water molecules.

JCAAA LANSFORDITE MgCO<sub>3</sub>·5H<sub>2</sub>O

JCAAB Open

JCAAC NESQUEHONITE Mg(HCO<sub>3</sub>)(OH) 2H<sub>2</sub>O mon/P2<sub>1</sub>/n

# **SERIES B**

**HELLERITE, Mon/2/c.** Structure not known. Williams, K.L., I.M. Threadgold, and A.W. Hounslow (1959) Hellyerite, a new nickel carbonate from Heazlewood, Tasmania. Amer. Mineral., 44, 533–538.

Threadgold, I.M. (1963) The crystal structure of hellyerite and nacrite. Dissertation Abs., 24(1), 252–253.

Anderson, P., et al. (2002): Famous mineral localities: The Lord Brassey mine, Tasmania. Mineralogical Record. 33, 321-332.

Bottrill, R. S. & Baker, W. E. (2008): A Catalogue of the Minerals of Tasmania. Geological Survey Bulletin 73, Mineral Resources Tasmania, 254 pp.

Powder Diffraction File: 24-523.

JCABA HELLERITE NiCO<sub>3</sub>·6H<sub>2</sub>O

# TYPE B CARBONATES WITH LARGE CATIONS (ALKALI AND ALKALI-REE)

### **SERIES A**

THERMONATRITE, orth/P2<sub>1</sub>ab. The structure is based on a distorted Na<sup>o</sup>[CI]<sup>c</sup> type structure, composed of [Na<sub>2</sub>(H<sub>2</sub>O)<sub>10</sub>]<sup>2+</sup> and CO<sub>3</sub> groups. The first group consists of two sodium-water octahedra that share an edge. These pairs of octahedra are linked by hydrogen bonds to form a three-dimensional framework. Structure consists of Na polyhedra sharing corners to form chains // [010];

the chains are linked into a framework by carbonate triangles that share an edge and a corner with the polyhedra.

JCBAA THERMONATRITE Na<sub>2</sub>CO<sub>3</sub>·H<sub>2</sub>O JCBAB NATRON Na<sub>2</sub>CO<sub>3</sub>·10H<sub>2</sub>O

JCBAC TRONA Na<sub>3</sub>(CO<sub>3</sub>)(HCO<sub>3</sub>)·2H<sub>2</sub>O

**SERIES B** 

MONOHYDROCALCITE. Trig/P3<sub>1</sub>. Structure consists of Ca polyhedra sharing two O-O edges with carbonate groups. In ikaite, the structure consists of discrete Ca carbonate groups, each of which is surrounded by an envelope of 18 water molecules. The revised structure of monohydrocalcite is composed of rods in which a spiral arrangement of Ca ions is accompanied by spiral arrangements of carbonate groups and water molecules.

JCBBA MONOHYDROCALCITE  $CaCO_3$ 'H $_2O$  hex/P3 $_1$ 12 JCBBB IKAITE  $CaCO_3$ '6H $_2O$  mon/C2/c or Cc

**SERIES C** 

PIRSSONITE, orth/Fdd2. Structure consists of Ca polyhedra sharing edges with two carbonate triangles to form a Ca carbonate unit; these units are linked into a framework by Na ions and water molecules which alternate to form chains // [011]. Structure consists of Ca polyhedra sharing edges with two carbonate triangles to form a Ca(CO<sub>3</sub>)<sub>2</sub> unit; these units are linked into a framework by Na ions and water molecules which alternate to form chains // [011]. In gaylussite, similar units are linked into a framework by Na atoms and H-bonding from the water molecules.

JCBCA PIRSSONITE Na<sub>2</sub>Ca(CO<sub>3</sub>)<sub>2</sub>·2H<sub>2</sub>O

JCBCB GAYLUSSITE  $Na_2Ca(CO_3)_2$ :5 $H_2O$  mon/C2/c or Cc

**SERIES D** 

CHALCONATRONITE, mon/P2<sub>1</sub>/n. Structure consist of sheets of face-sharing NaO<sub>6</sub> octahedra // (010) are connected by zigzag chains // [010] of corner-sharing Cu octahedra, each of which shares two edges with carbonate groups. Structure consists of sheets of face-sharing Na octahedra // (010) which are connected by zigzag chains // [010] of corner-sharing Cu octahedra, each of which shares two edges with carbonate groups. In baylissite, MgO<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub> octahedra share two edges with K polyhedra to form trimers that are linked by carbonate groups.

JCBDACHALCONATRONITE $Na_2Cu(CO_3)_2$ '3 $H_2O$  $mon/P2_1/a$ JCBDBBAYLISSITE $K_2Mg(CO_3)_2$ '4 $H_2O$  $mon/P2_1/a$ 

**SERIES E** 

TULIOKITE, trigonal/R3. The tuliokite structure consists of columns of face-sharing Ba and Th polyhedra // [001] which are connected into a framework by Na and H-bonding; the polyhedra share edges with six carbonate groups.

JCBEA TULIOKITE Na<sub>6</sub>BaTh(CO<sub>3</sub>)<sub>6</sub>·6H<sub>2</sub>O

**SERIES F** 

ALEXKHOMYAKOVITE, hex/P6<sub>3</sub>/mcm Pekov, I.V., Zubkova, N.V., Yapaskurt, V.O., Lykova, I.S., Chukanov, N.V., Belakovskiy, D.I., Britvin, S.N., Turchkova, A.G. and Pushcharovsky, D.Y. (2015) Alexkhomyakovite, IMA 2015-013. CNMNC Newsletter No. 25, June 2015, page 534; Mineralogical Magazine, 79, 529-535. The new mineral alexkhomyakovite K6(Ca2Na)(CO3)5CI · 6H2O (IMA2015-013) occurs in a peralkaline pegmatite at Mt. Koashva, Khibiny alkaline complex, Kola peninsula, Russia. It is a hydrothermal mineral associated with villiaumite, natrite, potassic feldspar, pectolite, sodalite, biotite. lamprophyllite, titanite, fluorapatite, wadeite, burbankite, rasvumite, djerfisherite, molybdenite and an incompletely characterized Na-Ca silicate. Alexkhomyakovite occurs as equant grains up to 0.2 mm, veinlets up to 3 cm long and up to 1 mm thick and fine-grained aggregates replacing delhayelite. Alexkhomyakovite is transparent to translucent, colourless, white or grey, with vitreous to greasy lustre. It is brittle, the Mohs hardness is ca. 3. No cleavage was observed, the fracture is uneven. Dmeas = 2.25(1), Dcalc = 2.196 g cm-3. Alexkhomyakovite is optically uniaxial (-),  $\omega = 1.543(2)$ ,  $\varepsilon = 1.476(2)$ . The infrared spectrum is reported. The chemical composition [wt%, electron microprobe data, CO2 and H2O contents calculated for 5 (CO3) and 6 (H2O) per formula unit (pfu), respectively] is: Na2O 4.09, K2O 35.72, CaO 14.92, MnO 0.01, FeO 0.02, SO3 0.11, CI 4.32, CO2 28.28, H2O 13.90, -O=CI -0.98, total 100.39. The empirical formula calculated on the basis of 9 metal

cations pfu is K5.90Ca2.07Na1.03(CO3)5(SO4)0.01O0.05Cl0.95 6H2O. The numbers of CO3 groups and H2O molecules are based on structure data. Alexkhomyakovite is hexagonal, P63/mcm, a 9.2691(2), c 15.8419(4) Å, V 1178.72(5) Å3 and Z = 2. The strongest reflections of the powder X-ray diffraction pattern [d Å(I)(hkl)] are: 7.96(27)(002), 3.486(35)(113), 3.011(100)(114), 2.977(32)(211), 2.676(36)(300), 2.626(42)(213, 115), 2.206(26)(311) and 1.982(17)(008). The crystal structure (solved from single-crystal X-ray diffraction data, R = 0.0578) is unique. It is based on (001) heteropolyhedral layers of pentagonal bipyramids (Ca,Na)O5(H2O)2 interconnected via carbonate groups of two types, edge-sharing ones and vertex-sharing ones. Ca and Na are disordered. Ten-fold coordinated K cations centre KO6Cl(H2O)3 polyhedra on either side of the heteropolyhedral layer. A third type of carbonate group and Cl occupy the interlayer. The mineral is named in honour of the outstanding Russian mineralogist Alexander Petrovich Khomyakov (1933–2012).

JCBFA ALEXKHOMYAKOVITE K<sub>6</sub>(Ca<sub>2</sub>Na)9CO<sub>3</sub>)<sub>5</sub>Cl.6H<sub>2</sub>O

TYPE C CARBONATES WITH REE.

SERIES A DONNAYITE SERIES, trig/R3m. The structure consists of six carbonate groups. Each group is very close to being planar and the usual equilateral triangles of oxygen atoms about each carbon are only slightly distorted. The water molecules have roughly tetrahedral coordination.

JCCAA WELOGANITE  $Na_2Sr_3Zr(CO_3)_6$ '3 $H_2O$  JCCAB DONNAYITE-(Y)  $NaCaYSr_3(CO_3)_6$ '3 $H_2O$ 

JCCAC MCKELVEYITE-(Y) Ba<sub>3</sub>Na(Ca,U)Y(CO<sub>3</sub>)<sub>6</sub>·3H<sub>2</sub>O tric/P<sub>1</sub>

JCCAD EWALDITE Ba(Ca,Y,Na)[CO<sub>3</sub>]<sub>2</sub> .  $nH_2O$ 

**SERIES B** 

TENGERITE SERIES, orth/Bb2<sub>1</sub>m. Structure consists of strips // [010] of corner-sharing YO<sub>8</sub>(H<sub>2</sub>O) polyhedra and edge-sharing carbonate groups // (001) forming corrugated pseudo-hexagonal sheets // (0010. In tengerite, these sheets are connected by carbonate groups // [001] to form a framework. The structure consists of a sheet structure built up from none-fold coordinated Y polyhedra and CO<sub>3</sub> trigonal planar groups. The corrugated sheets are connected by other CO<sub>3</sub> groups to form a three-dimensional framework. It is suggested that tengerite-(Y) has a close structural relationship to kimuraite-(Y) and lokkaite-(Y), whereas lanthanite-(La) is related to calkinsite-(Ce). The structure of shomiokite-(Y) is layered on (001), with Na(CO<sub>3</sub>).H<sub>2</sub>O layers being cross-linked by Y atoms in nine-coordination. This layer is comparable to a layer of similar composition in donnayite-(Y). The structure of galgenbertite-(Ce) is based on double layers // to (001), which are composed of Ca(1)Ce(2)(CO<sub>3</sub>)<sub>2</sub> single layers with an ordered chessboard like arrangement of Ca and Ce, and with a roof tile-like stacking of the carbonate groups. Perpendicular to (001) the double layers are connected to a triclinic framework structure with a good cleavage // to (0010) by a differently organized and more open part of the structure formed by Ce(3)(CO<sub>3</sub>)<sub>2</sub>(H<sub>2</sub>O).

JCCBA TENGERITE-(Y)  $Y_2(CO_3)_3 \cdot 2H_2O$ JCCBB KIMURAITE-(Y)  $CaY_2(CO_3)_4 \cdot 6H_2O$ JCCBC LOKKAITE-(Y)  $CaY_4(CO_3)_5 \cdot 9H_2O$ 

JCCBD GALGENBERGITE-(Ce) Ca(Ce,La,Nd)<sub>2</sub>(CO<sub>3</sub>)<sub>4</sub>.H<sub>2</sub>O JCCBE HIZENITE-(Y) Ca<sub>2</sub>Y<sub>6</sub>(CO<sub>3</sub>)<sub>11</sub>.14H<sub>2</sub>O

SERIES C SHOMIOKITE, orth/Pbn2<sub>1</sub>. Structure consists of YO<sub>9</sub> polyhedra sharing edges with 3 carbonate triangles, forming interrupted layers // (001), related to the layers found in donnayite; Na polyhedra are accommodated between the layers.

JCCCA SHOMIOKITE-(Y)  $Na_3Y(CO_3)_3$ :3H<sub>2</sub>O orth/Pbn2<sub>1</sub>

SERIES D LANTHANITE SERIES, orth/Pbnb. The structure consists of infinite layers // (010) of RE-O coordination polyhedra and CO<sub>3</sub> groups. These layers are parallel to the ac plane and are connected to one another only by H bonds. Structure consists of LaO<sub>6</sub>(H<sub>2</sub>O)<sub>4</sub> and LaO<sub>8</sub>(H<sub>2</sub>O)<sub>2</sub> polyhedra that are connected into sheets // (010) by carbonate groups.

JCCDA LANTHANITE-(La) (La,Ce)<sub>2</sub>(CO<sub>3</sub>)<sub>3</sub>·8H<sub>2</sub>O

JCCDB	LANTHANITE-(Nd)	$(Nd,La)_2(CO_3)_3\cdot 8H_2O$
JCCDC	LANTHANITE-(Ce)	(Ce,La) <sub>2</sub> (CO <sub>3</sub> ) <sub>3</sub> ·8H <sub>2</sub> O
JCCDD	LANTHANITE-(Y)	$(Y,La)_2(CO_3)_3$ ·8 $H_2O$
JCCDE	CALKINSITE-(Ce)	(Ce,La) <sub>2</sub> (CO <sub>3</sub> ) <sub>3</sub> ·4H <sub>2</sub> O

SERIES E DECRESPIGNYITE-Y, mon/P2/m, P2, or Pm. Structure not known. K. Wallwork, U. Kolitsch, A. Pring and

L. Nasdala (2002) Decrespignyite-(Y), a new copper yttrium rare earth carbonate chloride hydrate from Paratoo, South

Australia. Mineralogical Magazine: 66, 181-188.

JCCEA DECRESPIGNYITE-(Y) Cu(Y,REE)<sub>4</sub>(CO<sub>3</sub>)<sub>4</sub>Cl(OH)<sub>5</sub>·2H<sub>2</sub>O

GROUP D CARBONATES WITH ADDITIONAL ANIONS AND WATER.

TYPE A CARBONATES WITH MEDIUM-SIZED CATIONS.

SERIES A HYDROMAGNESITE. Mon/P2<sub>1</sub>/c. Structure consists of zigzag chains // [001] of edge-sharing MgO<sub>6</sub> octahedra which are connected into sheets // (140) by sharing corners with additional Mg

octahedra; the sheets are linked into a framework by carbonate groups.

 $\label{eq:JDAAA} JDAAA \qquad HYDROMAGNESITE \qquad Mg_5(CO_3)_4(OH)_2\cdot 4H_2O \qquad mon/P2_1/c$   $\label{eq:JDAAB} JDAAB \qquad DYPINGITE \qquad Mg_5(CO_3)_4(OH)_2\cdot 5H_2O \qquad mon/P2_1/c$   $\label{eq:JDAAC} JDAAC \qquad WIDGIEMOOLTHALITE \qquad (Ni,Mg)_5(CO_3)_4(OH)_2\cdot 4-5H_2O \qquad mon/P2_1/c$ 

JDAAD GIORGIOSITE  $Mg_5(CO_3)_4(OH)_2 \cdot 5H_2O$ 

SERIES B ARTINITE SERIES, mon/C2. Structure consists of edge-sharing MgO(OH)<sub>2</sub>(H<sub>2</sub>O)<sub>3</sub> octahedra forming

double chains // [010] with carbonate groups attached in a staggered arrangement on either side of the double chains; these chains, together with four other chains along [100] and [001], are connected into a framework by H-bonding (from OH and water). The structure is based on the packing of  $CO_3$ ,

H₂O and OH ions. Mg atoms occupy voids in this packing with octahedral coordination.

JDABA ARTINITE Mg<sub>2</sub>(CO<sub>3</sub>)(OH)<sub>2</sub>·3H<sub>2</sub>O mon/C2

JDABB CHLORARTINITE  $Mg_2(CO_3)CI(OH)^3H_2O$ JDABC INDIGIRITE  $Mg_2Al_2(CO_3)_4(OH)_2^15H_2O$ 

SERIES C OTWAYITE Structures not known. Silliman (1847) American Journal of Science: 3: 407 (as Hydrate of

Nickel).

Silliman (1848) American Journal of Science: 6: 248 (as Emerald Nickel).

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Casares (1851) A.M. Alcibar in Min. Revista of Madrid: 176, March, 1851 (as Zaratita).

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679: 158.

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Fenoglio M. – (1934) Nuove ricerche sulla zaratite: zaratite sintetica. Periodico di Mineralogia - Roma pp. 265-274.

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Mineralogical Magazine (1963): 33: 663.

Garcia-Guinea, J., La Iglesia, A., Crespo-Feo, E., González del Tanago, J., Correcher, V. (2014): The status of zaratite; investigation of the type specimen from Cape Ortegal, Galicia, Spain. European Journal of Mineralogy, 25, 995-1004.

Nickel, E. H., Robinson, B. W., Davis, C. E. S. & MacDonald, R. D. (1977): Otwayite, a new nickel mineral from Western Australia. American Mineralogist: 62: 999-1002.

Nickel, E. H. & Graham, J. (1987): Paraotwayite. A new nickel hydroxide mineral from Western Australia. Canadian Mineralogist: 25: 409-411.

JDACAZARATITE $Ni_3(CO_3)(OH)_4\cdot 4H_2O$ JDACBOTWAYITE $(Ni,Mg)_2(CO_3)(OH)_2\cdot H_2O$ JDACCPARAOTWAYITE $Ni(OH)_{1.4}(SO_4,CO_3)_{0.3}$ 

#### **SERIES D**

KAMBALDAITE, hex/P63. The structure consists of distorted NiO6 octahedra which are linked in a three-dimensional edifice with bridging carbonate and hydroxyl groups. Columnar tunnels through the structure are occupied by arrays of Na atoms with octahedral environments of bridging water molecules. The structure of szymanskiite shows some similarities to that of kambaldaite. Basically, the structure is composed of two separate components. The first, is an octahedrally coordinated (Ni.Mq) cationic group bonded to oxygen atoms, connected to symmetry-related octahedra, adjacent to z, by means of O(2)-O(3) edge-sharing hydroxyl groups. A second link between adjacent octahedra is found in the form of an ordered carbonate group. This group spans from oxygen O(4) of one octahedron to oxygen O(5) of the adjacent octahedron. The third oxygen atom O(1) of the carbonate group is involved in a most unusual Hg<sup>1+</sup> chain. The two atoms Hg(1) and Hg(2) overlap in the z-projection and the pairs of Hg atoms are separated from each other by a face of three O(1) oxygen atoms. The (Ni,Mg) octahedra edge-share to adjacent octahedra; the carbonate cation bridges two octahedra in z; the two tetrahedrally coordinated mercury atoms link carbonate groups adjacent to z; finally, the trigonal prismatic blocks themselves share edges along z. A framework structure of very rigid tubes is thus formed, with the tubes strongly held together. Structure consists of chains of edge-sharing NiO<sub>6</sub> and NiO<sub>3</sub>(OH)<sub>3</sub> octahedra // [0001] which are connected into large tubes // [0001] by sharing edges and corners of octahedra, and strengthened by carbonate groups; the tubes // [0001] contain chains of face-sharing Na(H₂O)<sub>6</sub> octahedra.

JDADA KAMBALDAITE NaNi<sub>4</sub>(CO<sub>3</sub>)<sub>3</sub>(OH)<sub>3</sub>·3H<sub>2</sub>O

# **SERIES E**

CALLAGHANITE, mon/C2/c. Structure consists of zigzag chains of edge-sharing Mg octahedra // [101] which are linked by carbonate groups and pairs of edge-sharing Cu pyramids; the carbonate triangles are // (001).

JDAEA CALLAGHANITE  $Cu_2Mg_2(CO_3)(OH)_6$ :2 $H_2O$ 

## **SERIES F**

CLARAITE, tric/P1. The structure has a layered motif, with  $\{001\}$  heteropolyhedral layers formed by  $Cu_5$  and  $Cu_6$  polyhedra as well as As a and Carbonate groups. These layers are stacked along c through edge-sharing  $Cu_2O_{10}$  and  $Cu_2O_{8}$  dimers. Walenta, K. (1982): Clarait, ein neues Karbonatmineral aus der Grube Clara (mittlerer Schwarzwald). Chem. Erde, 41, 97-102. (in German).

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Putz, H., Lechner, A. & Poeverlein, R. (2012): Erythrin und Clarait vom Pichlerstollen am Silberberg bei Rattenberg, Nordtirol. Lapis, 37 (1), 47-52; 62 (in German). [also on U184 = claraite and U130 = claraite]

**JDAFA CLARAITE**  $(Cu,Zn)_{15}(CO_3)_4(AsO_4)_2(SO_4)(OH)_{14}.7H_2O$ 

**SERIES G** SCARBROITE, tric/P1 or P1. Structure not known. American Mineralogist (1958): 43: 384.

Mineralogical Magazine (1980): 43: 615-618.

**JDAGA SCARBROITE**  $AI_{5}[(OH)_{13}/CO_{3}]$ .  $5H_{2}O$ **JDAGB HYDROSCARBROITE** Al<sub>14</sub>(CO<sub>3</sub>)<sub>3</sub>(OH)<sub>36</sub> nH<sub>2</sub>O

**SERIES H** QUINTINITE SERIES, related to the MANASSEITE-HYDROTALCITE Structure series.

**JDAHA** QUINTINITE-2H, 3T  $Mg_4Al_2(OH)_{12}CO_3 \cdot 3H_2O$ (Group)

**JDAHB** open

**JDAHC** CHARMARITE-2H, 3T  $Mn_4Al_2(OH)_{12}CO_3 \cdot 3H_2O$ 

**JDAHD** open

**JDAHE CARESITE-3T** Fe<sub>4</sub>Al<sub>2</sub>(OH)<sub>12</sub>CO<sub>3</sub>·3H<sub>2</sub>O **JDAHF ZACCAGNAITE** Zn<sub>4</sub>Al<sub>2</sub>(OH)<sub>12</sub>CO<sub>3</sub>·3H<sub>2</sub>O

**SERIES I** MANASSEITE-HYDROTALCITE SERIES, hex/P63/mmc; trig/R3m or R3m. Structure consists of brucite-like layers // (0001) of edge-sharing octahedra of divalent and trivalent cations alternate with

layers containing water molecules and charge-balancing anions.

**JDAIA** Mg<sub>6</sub>Al<sub>2</sub>(CO<sub>3</sub>)(OH)<sub>16</sub>·4H<sub>2</sub>O (2H polytype of hydrotalcite) MANASSEITE (D)

**JDAIB** BARBERTONITE (D) Mg<sub>6</sub>Cr<sub>2</sub>(CO<sub>3</sub>)(OH)<sub>16</sub> 4H<sub>2</sub>O (2H polytype of pyroaurite)

**JDAIC** SJÖGRENITE (D)  $Mg_6Fe_2(CO_3)(OH)_{16} \cdot 4H_2O$  (2H polytype of stichtite)

**JDAID HYDROTALCITE**  $Mg_6Al_2(CO_3)(OH)_{16} 4H_2O$  (Group)

**JDAIE STICHTITE** Mg<sub>6</sub>Cr<sub>2</sub>(CO<sub>3</sub>)(OH)<sub>16</sub> 4H<sub>2</sub>O **JDAIF PYROAURITE**  $Mg_6Cr_2(CO_3)(OH)_{16} \cdot 4H_2O$ **JDAIG**  $Mg_6Mn_2(CO_3)(OH)_{16} 4H_2O$ **DESAULTELSITE JDAIH REEVESITE** Ni<sub>6</sub>Fe<sub>2</sub>(CO<sub>3</sub>)(OH)<sub>16</sub>·4H<sub>2</sub>O **JDAII TAKOVITE** Ni<sub>6</sub>Al<sub>2</sub>(CO<sub>3</sub>)(OH)<sub>16</sub>·4H<sub>2</sub>O **JDAIJ COMBLAINITE** Ni<sub>6</sub>Co<sub>2</sub>(CO<sub>3</sub>)(OH)<sub>16</sub>·4H<sub>2</sub>O **JDAIK COALINGITE** Fe<sub>2</sub>Mg<sub>10</sub>(CO<sub>3</sub>)(OH)<sub>24</sub>·2H<sub>2</sub>O **JDAIL BRUGNATELLITE**  $Mg_6Fe(CO_3)(OH)_{13} \cdot 4H_2O$ 

**JDAIM CHLORMAGALUMINITE** (Mg,Fe)<sub>4</sub>Al<sub>2</sub>(OH)<sub>12</sub>(Cl<sub>2</sub>,CO<sub>3</sub>) 2H<sub>2</sub>O

**JDAIN** WERMLANDITE (Ca,Mg)Mg<sub>7</sub>(Al,Fe)<sub>2</sub>(SO<sub>4</sub>)<sub>2</sub>(OH)<sub>18</sub>·12H<sub>2</sub>O

**JDAIO SHIGAITE** NaMn<sub>6</sub>Al<sub>3</sub>(SO<sub>4</sub>)<sub>2</sub>(OH)<sub>18</sub>·12H<sub>2</sub>O

**JDAIP MOTUKOREAITE**  $Na_{0.6}(Al_{3.4}Mg_{5.6})(SO_4)_{1.3}(CO_3)_{0.7}(OH)_{18} \cdot 12H_2O$ 

**JDAIQ NIKISCHERITE**  $NaFe^{2+}_{6}Al_{3}(SO_{4})_{2}(OH)_{18}(H_{2}O)_{12}$ 

 $Mg_6Cr_2(OH)_{16}Cl_2^{-1}4H_2O$ **JDAIR** WOODALLITE

**JDAIS KARCHEVSKYITE**  $[Mg_{18}AI_{9}(OH)_{54}][Sr_{2}(CO_{3},PO_{4})_{9}(H_{2}O,H_{3}O)_{11}]$ 

Ni<sub>3</sub>Fe<sup>3+</sup>Cl(OH)<sub>8</sub>.2H<sub>2</sub>O **JDAIT DRONINOITE**  $(Ni,Cu)_2Fe^{3+}(OH)_6[Sb(OH)_6]$ **JDAIU OMSITE** 

**SERIES J** CYANOTRICHITE SERIES, orth/. /. Structure consists of edge-sharing octahedral ribbons Cu<sub>2</sub>Al(O,HO,H<sub>2</sub>O)<sub>8</sub> form H-bonded layers // to (001), as in khaidarkanite. The partially occupied interlayer Sb and S sites of the average structure are in octahedral and tetrahedral coordination bhy O, respectively. They cannot be occupied simultaneously, which leads to regular alternation of

[Sb(OH)<sub>6</sub>-SO<sub>4</sub> groups in rods // y, resulting in local tripling of the periodicity along y for the Sb(OH)<sub>6</sub>-SO<sub>4</sub>rods. Thus, camerolaite has a 'host-guest' structure in which an invariant host module (layers of Cu-Al ribbons) has embedded rod-like guest modules with a longer periodicity.

JDAJA CARBONATECYANOTRICHITE Cu<sub>4</sub>Al<sub>2</sub>(CO<sub>3</sub>,SO<sub>4</sub>)(OH)<sub>12</sub>·2H<sub>2</sub>O LDDBA CYANOTRICHITE Cu<sub>4</sub>Al<sub>2</sub>(SO<sub>4</sub>)(OH)<sub>12</sub>·2H<sub>2</sub>O

LDDBB CAMEROLAITE Cu<sub>4</sub>Al<sub>2</sub>(HSbO<sub>4</sub>,SO<sub>4</sub>)(CO<sub>3</sub>)(OH)<sub>10</sub><sup>-</sup>2H<sub>2</sub>O mon/P2<sub>1</sub> or P2<sub>1</sub>/m

**SERIES K** 

NIVEOLANITE, tetr/P4/mcc. The structure includes isolated, infinite chains of BeO<sub>2</sub>(OH)<sub>2</sub> tetrahedra linked via common OH groups: two other vertices of each Be tetrahedron are shared with carbonate groups, and Na cations occupy seven-fold polyhedra [NaO<sub>6</sub>(H<sub>2</sub>O)] forming columns. Chains of Be tetrahedra and columns of Na polyhedra are aligned along the c axis, just as broad channels in which water molecules are located

JDAKA NIVEOLANITE NaBe(CO<sub>3</sub>)(OH).2H<sub>2</sub>O

SERIES L

PUTNISITE, orth/Pnma. The structure consists of  $Cr(OH)_4O_2$  octahedra linked by edge-sharing to form an eight-membered ring. A 10-coordinated Sr cation lies at the center of each ring. The rings are decorated by carbonate triangles, each of which links by corner-sharing to two  $Cr(OH)_4O_2$  octahedra. Rings are linked by  $Ca(H_2O)_4O_4$  polyhedra to form a sheet // to (100). Adjacent sheets are joined along [100] by corner-sharing  $SO_4$  tetrahedra. Water molecules occupy channels that run along [100] and interstices between slabs.

JDALA PUTNISITE SrCa<sub>4</sub>Cr<sup>3+</sup><sub>8</sub>(CO<sub>3</sub>)<sub>8</sub>SO<sub>4</sub>(OH)<sub>16</sub>.23H<sub>2</sub>O

**SERIES M** 

MARKLITE, mon/P2<sub>1</sub>/c. The structure contains four Cu, one C, nine O and nine H sites in the asymmetric unit. The Cu1, Cu2 and Cu3 sites are coordinated by six ligands, including O and OH, and linked to form the infinite sheet of edge-sharing distorted Cu-octahedra, of the composition {Cu<sup>2+</sup><sub>4</sub>O<sub>2</sub>(OH)<sub>6</sub>} // to (100). Adjacent infinite sheets are separated by the periodicity of a and are linked through the interstitial complex. This complex consists of a distorted Cu tetragonal bipyramid with two water ligands and is chelated by two carbonate groups which link them into the framework an additional four water groups are localized in the interstitual positions providing linkage. The structure is related to both hydrozincite and auraichalcite.

JKAMA MARKLITE  $Cu_5(CO_3)_2(OH)_6.6H_2O$ 

SERIES N SLIKITE, tric/P1.

JKANA SLIKITE  $Zn_2Mg(CO_3)_2(OH)_2.4H_2O$ 

TYPE B CARBONATES WITH LARGE AND MEDIUM-SIZED CATIONS.

SERIES A ALUMOHYDROCALCITE, tric/P1. Stachowicz, M., Parafiniuk, J., Wilson, C., Coles, S. & Woźniak, K.

(2015): Applications of Hirshfeld surfaces to mineralogy: An example of alumohydrocalcite, and the

classification of the dundasite group minerals. American Mineralogist, 100, 110-119.

JDBAA ALUMOHYDROCALCITE CaAl<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>4</sub>· 4H<sub>2</sub>O JDBAB PARA-ALUMOHYDROCALCITE CaAl<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>4</sub>· 6H<sub>2</sub>O

**SERIES B** 

HYDRODRESSERITE SERIES, tric/P1. Barium is coordinated by nine oxygen atoms. Al coordination is distorted octahedral, with four OH groups in a square, and two carbonate oxygen atoms trans to each other. Carbonate ions bind the aluminum atoms into zigzag ribbons. The metal coordination is very similar to that found in dundasite. An extensive network of H bonds (interhydroxyl, hydroxyl, water and water-carbonate oxygen) holds the elements of the structure together. Structure consists of edge-sharing AlO<sub>2</sub>(OH)<sub>4</sub> octahedra and PbO<sub>8</sub>(OH) polyhedra linked by 3 shared O atoms forming chains along [001]; both types of polyhedra are connected into a framework by common O and carbonate groups.

JDBBA HYDRODRESSERITE SrAl<sub>2</sub>(CO<sub>3</sub>)<sub>2</sub>(OH)<sub>4</sub>· 3H<sub>2</sub>O

JDBBBDUNDASITE $PbAl_2(CO_3)_2(OH)_4$ · $H_2O$ JDBBCDRESSERITE $BaAl_2(CO_3)_2(OH)_4$ · $1.5H_2O$ JDBBDSTRONTIODRESSERITE $SrAl_2(CO_3)_2(OH)_4$ · $H_2O$ 

JDBBE MONTROYALITE Sr<sub>4</sub>Al<sub>8</sub>(CO<sub>3</sub>)<sub>3</sub>(OH,F)<sub>26</sub>·10H<sub>2</sub>O (may be related to the dundasite group)

JDBBFPETTERDITE $PbCr_2(CO_3)_2(OH)_4$   $H_2O$ JDBBGKOCHSANDORITE $CaAl_2(CO_3)_2(OH)_4$   $H_2O$ 

SERIES C SZYMANSKIITE, hex/P63. Structure consists of chains of [-O-Hg-Hg-O-] chains of Hg atoms and trios

of O atoms in a face-sharing column of the form [-Hg-O $_3$ -Hg-Hg-O $_3$ -Hg], and distorted (Ni,Mg)O $_6$  octahedra, connected by carbonate groups. Large channels contain disordered components of the

structure.

JDBCA SZYMANSKIITE Hg<sub>16</sub>(Ni,Mg)<sub>6</sub>(CO<sub>3</sub>)<sub>12</sub>(OH)<sub>12</sub>(H<sub>3</sub>O)<sub>8</sub>·3H<sub>2</sub>O

SERIES D SCHUILINGITE, orth/P21cn. Structure not known. Vaes (1947) Société géologique de Belgique, Bulletin,

Liége: 70: 233.

Palache, C., Berman, H., & Frondel, C. (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: 252.

American Mineralogist (1958): 43: 796.

Canadian Mineralogist (1999): 37: 1463-1470.

Leverett, P.L. & P.A.Williams, Schuilingite-(Nd) from the Peelwood mine, Peelwood, New South Wales,

Australian J. Mineralogy 13(2), 89-91 (2007)

JDBDA SCHUILINGITE-(Nd) CuPb(Nd,Gd,Sm)(CO<sub>3</sub>)(OH)<sup>·</sup>0.5H<sub>2</sub>O

SERIES E SERGEEVITE, trig/. Structure not known but may be near that of huntite. American Mineralogist

(1981): 66: 1100.

Zapiski Vserossiyskogo Mineralogicheskogo Obshchestva: 109(2): 217-223.

JDBEA SERGEEVITE  $Ca_2Mg_{11}(CO_3)_{13}$  .  $10H_2O$ 

TYPE C CARBONATES WITH LARGE CATIONS.

SERIES A ANCYLITE SERIES, orth/Pmcn. The structure can ideally be derived from that of the orthorhombic

carbonates by introducing in the latter a hydroxyl group lying on the mirror plane and bonded to the heavy cations. The introduction of the OH groups in the compact aragonite structure results in the relative shifts of the two superposed carbonate ions and in the angle of tilt between the CO<sub>3</sub> triangle

and the ab plane.

JDCAA ANCYLITE-(Ce)  $SrCe(CO_3)_2(OH)^{\cdot}H_2O$ 

JDCAB CALCIO-ANCYLITE-(Ce)  $(Ca,Sr)Ce(CO_3)_2(OH)^{\cdot}H_2O$ 

JDCAC CALCIO-ANCYLITE-(Nd) (Ca,Sr)(Nd,Ce)(CO<sub>3</sub>)<sub>2</sub>(OH)·H<sub>2</sub>O

JDCAD GYSINITE-(Nd)  $(Nd,Pb)CO_3(OH,H_2O)$ JDCAE ANCYLITE-(La) SrLa( $CO_3$ )<sub>2</sub>(OH)<sup>-</sup>H<sub>2</sub>O

JDCAF KOZOITE-(Nd)  $Nd(CO_3)()OH)$ JDCAG KOZOITE-(La)  $La(CO_3)(OH)$ 

SERIES B KAMPHAUGITE, tetr/P4<sub>1</sub>2<sub>1</sub>2. Structure consists of Ca and Y polyhedra sharing edges, corners and

faces with each other, and edges with carbonate groups to form corrugated sheets // (001); the

sheets are connected by sharing oxygens of the polyhedra.

SERIES C SHELDRICKITE, trig/P3<sub>2</sub>. Structure consists of sheets // (0001) of Na polyhedra, carbonate triangles

and water molecules alternating with sheets containing Ca polyhedra and F ions; the carbonate groups are oriented  $\perp$  (0001), as in bastnasite. The structure is based on layering on (001). One layer consists of  $(CO_3)^2$  groups oriented perpendicular to (001), the  $Na\phi_8$  polyhedra and the water groups. A second layer consists of  $Ca\phi_9$  polyhedra and F anions. The structure of sheldrickite bears little resemblance to the chemically similar roubilleite, but it seems to be a modification of the structures

of bastnäsite and cebaite.

JDCCA SHELDRICKITE NaCa<sub>3</sub>(CO<sub>3</sub>)<sub>2</sub>F<sub>3</sub>.H<sub>2</sub>O

SERIES D THOMASCLARKITE-(Y), mon/P2. Structure consists of layers // (010) of edge-sharing Y and Na

polyhedra with attached carbonate groups which are linked by a sheet of water molecules The structure is layered on {010}. One layer consists of [HCO $_3$ ] groups oriented perpendicular to (010) and H-bonded to a water layer. A second layer consists of (Y $\Phi_8$ ) polyhedra and (Na $\Phi_6$ ) polyhedra

which are H-bonded to the water layer.

JDCDA THOMASCLARKITE-(Y) Na(Y,REE)(HCO<sub>3</sub>)(OH)<sub>3</sub>.4H<sub>2</sub>O

JDCDB ADAMSITE-(Y) NaY(CO<sub>3</sub>)<sub>2</sub>.6H<sub>2</sub>O

SERIES E PETERBAYLISSITE, orth/Pcab.

JDCEA PETERBAYLISSITE Hq<sub>3</sub>(CO<sub>3</sub>)(OH)<sup>2</sup>H<sub>2</sub>O (May not be a carbonate)

JDCEB CLEARCREEKITE Hg<sub>3</sub>(CO<sub>3</sub>)(OH)<sup>2</sup>H<sub>2</sub>O mon/P2<sub>1</sub>/c

SERIES F LUSERNAITE, orth/Pmna. The structure is built by layers // to (010), formed by chains of edge-

sharing Y-centered polyhedral (Y1), which run along [100], and are connected along c through Alcentered octahedral. These chains are decorated on one side by corner-sharing chains of Y-centered polyhedral (Y2), and on the other side by CO<sub>3</sub> groups. Along [001] the decorated chains

alternate their polarity.

JDCFA LUSERNAITE-(Y) Y<sub>4</sub>AI(CO<sub>3</sub>)<sub>2</sub>(OH,F)<sub>11</sub>.6H<sub>2</sub>O

GROUP E URANYL CARBONATES

TYPE A URANYL CARBONATES WITH UO<sub>2</sub>:CO<sub>3</sub> = 1:1

SERIES A RUTHERFORDINE, orth/Pmmm. Structure consists of UO2 groups are perpendicular to (010) and

equatorially surrounded by six O atoms belonging to four carbonate groups; the apices of the carbonate triangles are directed alternately in the +c and -c directions in successive sheets.

JEAAA RUTHERFORDINE UO<sub>2</sub>(CO<sub>3</sub>)

SERIES B BLATONITE, hex/. Structure not known. Canadian Mineralogist: 36: 1077-1081.

JEABA BLATONITE UO2CO3·H2O

SERIES C JOLIOTITE, orth/. Structure not known. Walenta, K. (1976): Widenmannit und Joliotit, zwei neue

Uranylkarbonatmineralien aus dem Schwarzwald. Schweiz. Mineral. Petrog. Mitt., 56, 167-185 (in German

with English abs.).

Mineralogical Abstracts (1977): 28: 208.

JEACA JOLIOTITE (UO<sub>2</sub>)CO<sub>3</sub>·2H<sub>2</sub>O

SERIES D BIJVOETITE, orth/C2ma, Cmb2 or Cmma. Structure consists of dimmers of edge-sharing UO<sub>265</sub>

pentagonal dipyramids alternating with dimmers of  $UO_{2\phi}$  hexagonal dipyramids to form strong chains // [100]; these are decorated on both sides by carbonate groups, and cross-linked by Y polyhedra to form sheets // (010), with 14 interlayer water molecules pfu. Structure of kamotoiite-(Y) consists of electroneutral sheets of the bijvoetite-(Y) uranylanion-topology and an interlayer with

water molecules not-coordinated directly to any metal cation

JEADA BIJVOETITE-(Y)  $(Y,Dy)_2(UO_2)_4(CO_3)_4(OH)_6$ :11H<sub>2</sub>O

JEADB KAMOTOITE-(Y)  $Y_2O_4(UO_2)_4(CO_3)_3$ ·14H<sub>2</sub>O

TYPE B URANYL CARBONATES WITH UO<sub>2</sub>:CO<sub>3</sub> = <1:1 – 1:2

SERIES A FONTANITE, orth/P2<sub>1</sub>nm. Structure not known. New Minerals (1997), New Minerals 1990-1994.

European Journal of Mineralogy: 4: 1271-1274.

Hughes, K.-A. and Burns, P.C. (2003a) A new uranyl carbonate sheet in the crystal structure of fontanite, Ca[(UO2)3(CO3)2O2](H2O)6. American Mineralogist: 88: 962-966.

Burns, P.C. (2005) U 6+ minerals and inorganic compounds: insights into an expanded structural hierarchy of crystal structures. Canadian Mineralogist; 43: 1839-1894.

JEBAA FONTANITE Ca(UO<sub>2</sub>)<sub>3</sub>(CO<sub>3</sub>)<sub>4</sub>·3H<sub>2</sub>O

SERIES B METAZELLERITE, orth/Pbna or Pbn2<sub>1</sub>. Structures not known. New Mexico Bur. Mines Resources, Mem. (1963): 15: 21.

American Mineralogist (1966): 51: 1567-1578. The structure of meyrowitzite contains both UO<sub>7</sub> pentagonal bipyramids and UO<sub>8</sub> hexagonal bipyramids, the latter participating in uranyl tricarbonate clusters (UTC). The two kinds of bipyramids and the carbonate groups link to form a novel corrugated heteropolyhedral sheet. The meyrowitzite structure is not identical with that of zellerite but it is placed here because of the U:C ratio of 1:2. Meyrowitzite, Ca(UO2)(CO3)2-5H2O, is a new mineral species from the Markey mine, Red Canyon, San Juan County, Utah, U.S.A. It is a secondary phase found on calcite-veined asphaltum in association with gypsum, markevite, and rozenite. Meyrowitzite occurs as blades up to about 0.2 mm in length, elongate on [010], flattened on {100}, and exhibiting the forms (100), (001), (101), (110), and (011). The mineral is yellow and transparent with vitreous luster and very pale yellow streak. Fluorescence under a 405 nm laser is from weak greenish yellow to moderate greenish blue. The Mohs hardness is ca. 2, tenacity is brittle, fracture is irregular, and there is one perfect cleavage, {101}. The measured density is 2.70(2) g/cm3. The mineral is optically biaxial (+) with  $\alpha$  = 1.520(2),  $\beta$  = 1.528(2), and  $\gamma$  = 1.561(2) (white light). The 2V(meas) = 53.0(6)°; weak dispersion, r > v; optical orientation: Z = b, Y ^ a ≈ 19° in obtuse β; pleochroism pale yellow, X ≈ Y < Z. Electron microprobe analyses provided the empirical formula Ca0.94(U1.00O2)(CO3)2-5(H2.02O) on the basis of U = 1 and O = 13 apfu, as indicated by the crystal structure determination. Meyrowitzite is monoclinic, P21/n, a = 12.376(3), b = 16.0867(14), c = 20.1340(17) Å,  $\beta$  = 107.679(13)°, V = 3819.3(12) Å3, and Z = 12. The structure (R1 = 0.055 for 3559 lo > 201) contains both UO7 pentagonal bipyramids and UO8 hexagonal bipyramids, the latter participating in uranyl tricarbonate clusters (UTC). The two kinds of bipyramids and the carbonate groups link to form a novel corrugated heteropolyhedral sheet. This is the first structural characterization of a uranyl-carbonate mineral with a U:C ratio of 1:2. Meyrowitzite is apparently dimorphous with zellerite.

JEBBAMETAZELLERITE $Ca(UO_2)(CO_3)_2$ '3 $H_2O$ orth/Pbn21 or PbnmJEBBBZELLERITE $Ca(UO_2)(CO_3)_2$ '5 $H_2O$ orth/Pmmm or Pmn21JEBBCMEYROWITZITE $Ca(UO_2)(CO_3)_2$ .5 $H_2O$ mon/P21/n

SERIES C EWINGITE, tetr/l4<sub>1</sub>/acd. The structure of ewingite is built from two smaller cluster motifs known to occur in other uranyl-carbonate minerals and synthetic phases. Each cluster is composed of 12 uranyl carbonates units, and four trinuclear [(UO<sub>2</sub>)<sub>3</sub>O(OH)<sub>3</sub>]<sup>+</sup> units for a total of 24 U polyhedra, with 2 Mg and 6 Ca occurring inside the cage. Trinuclear units share a common central vertex, and coordinated to another through Ca cations. Additional linkages are made to other trinuclear units by sharing apices of carbonate triangles of the uranyl dicarbonate and tricarbonate units.

JEBCA EWINGITE Mg<sub>8</sub>Ca<sub>8</sub>(UO<sub>2</sub>)<sub>24</sub>(CO<sub>3</sub>)<sub>30</sub>O<sub>4</sub>(OH)<sub>12</sub>(H<sub>2</sub>O)<sub>138</sub>

TYPE C URANYL CARBONATES WITH UO<sub>2</sub>:CO<sub>3</sub> = 1:3

SERIES A BAYLEYITE, mon/P2<sub>1</sub>/a. Structure consists of two insular Mg octahedra, on insular [UO<sub>2</sub>/(CO<sub>3</sub>)<sub>3</sub>]<sup>4</sup>-

unit, and six free water molecules which are linked only by H bonding; the plane of the uranyl-

carbonate unit is about // (001).

JECAA BAYLEYITE Mg<sub>2</sub>(UO<sub>2</sub>)(CO<sub>3</sub>)<sub>3</sub>·18H<sub>2</sub>O mon/P2<sub>1</sub>/a

SERIES B SWARTZITE, mon/P2<sub>1</sub>/m. Structure consists of one insular Mg octahedra and one CaO<sub>2</sub>(H<sub>2</sub>O)<sub>6</sub>

polyhedron which is edge-connected by a [UO<sub>2</sub>/(CO<sub>3</sub>)<sub>3</sub> unit, and are linked only by H-bonding. The

plane of the uranyl-carbonate unit is about perpendicular to [001].

JECBA SWARTZITE  $CaMg(UO_2)(CO_3)_3\cdot 12H_2O$   $mon/P2_1/m$ 

SERIES C ALBRECHTSCHRAUFITE, tric/P1. One MgF<sub>2</sub>O<sub>3</sub>(H<sub>2</sub>O) octahedron and three Ca polyhedra form

sheets // (100) with a  $[UO_2/(CO_3)_3]^4$  unit, the sheets are interconnected by another uranyl unit, four

free water molecules and H-bonding.

JECCA ALBRECHTSCHRAUFITE Ca<sub>4</sub>Mq(UO<sub>2</sub>)<sub>2</sub>(CO<sub>3</sub>)<sub>6</sub>F<sub>2</sub>·17H<sub>2</sub>O tric/P1 or P1

SERIES D LIEBIGITE, orth/Bba2. [UO<sub>2</sub>/(CO<sub>3</sub>)<sub>3</sub>]<sup>4-</sup> units are connected by CaO<sub>4</sub>(H<sub>2</sub>O)<sub>4</sub> polyhedra to form zigzag

chains // [001], and by CaO<sub>4</sub>(H<sub>2</sub>O)<sub>4</sub> polyhedra to form straight chains // [100]; this results in puckered

sheets // (010); between the sheets are three free water molecules, with only H-bonding

JECDA LIEBIGITE Ca<sub>2</sub>(UO<sub>2</sub>)(CO<sub>3</sub>)<sub>3</sub>·10H<sub>2</sub>O orth/Bba2

SERIES E RABBITTITE, mon/. Structure not known. American Mineralogist (1955): 40: 201-206.

JECEA RABBITTITE Ca<sub>3</sub>Mg<sub>3</sub>(UO<sub>2</sub>)<sub>2</sub>(CO<sub>3</sub>)<sub>6</sub>(OH)<sub>4</sub> 18H<sub>2</sub>O

SERIES F ANDERSONITE, trig/R3m. Structure consists of two NaO<sub>4</sub>(H<sub>2</sub>O)<sub>2</sub> octahedra, one Ca polyhedron one

[UO<sub>2</sub>/(CO<sub>3</sub>)<sub>3</sub>]<sup>4-</sup> unit and five water molecules per formula unit to form a framework with wide channels // [0001] that accommodate water; the plane of the uranyl-carbonate units is about perpendicular to

(0001).

JECFA ANDERSONITE Na<sub>2</sub>Ca(UO<sub>2</sub>)(CO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O

SERIES G GRIMSELITE, hex/P62c. The structure is similar to that of andersonite, except that the plane of the

uranyl-carbonate units is parallel to (0001). The presence of Na atoms in KO<sub>8</sub> polyhedra, which are

located in channels in the sructures.

JECGA GRIMSELITE K<sub>3</sub>Na(UO<sub>2</sub>)(CO<sub>3</sub>)<sub>3</sub>·H<sub>2</sub>O

SERIES H WIDENMANNITE, orth/Pmmn Structure of widenmannite is unique among the uranyl carbonates and

U<sup>6+</sup> compounds in general. The structure has corner sharing of UO<sub>8</sub> hexagonal bipyramids, forming infinite chains along [100]. One CO<sub>3</sub> group is bidentately linked to two adjacent bipyramids, while the second carbonate group is staggered at the opposite edge of each bipyramid. Adjacent UO<sub>8</sub> chains are occasionally interrupted by a vacancy, and linked th rough a (U2)O<sub>8</sub> bipyramid, which is attached to the chains by corner sharing of equatorial O(2) and O(4) atoms and edge sharing with carbonate groups. It is apparent that the widenmannite topology can be derived from that of

rutherfordine by a relative shift of every second row.

JECHA WIDENMANNITE  $Pb_2(OH)_2[(UO_2)(CO_3)_2]$ 

SERIES I ZNUCALITE, tric/P1. Structure not known. Neues Jahrbuch für Mineralogie, Monatshefte (1990): 393-400.

American Mineralogist (1994): 79: 1214.

New Minerals (1997) New Minerals 1990-1994.

JECIA ZNUCALITE  $Zn_{12}(UO_2)Ca(CO_3)_3(OH)_{22}$ · $4H_2O$ 

SERIES J CEJKAITE, Tri, P1 or P1. Structure consists of a [UO<sub>2</sub>O<sub>6</sub>] skeleton with almost linear O-U-O that is

roughly perpendicular to an irregular cycle formed by six O atoms that, in turn, belong to three more-or-les regular and planar CO<sub>3</sub> groups. Atoms Na1, Na1a and Na2 are octahedrally coordinated,

whereas Na3 is pentagonally coordinated.

JECJA CEJKAITE Na<sub>4</sub>(UO<sub>2</sub>)(CO<sub>3</sub>)<sub>3</sub>

JECJB AGRICOLAITE K<sub>4</sub>(UO<sub>2</sub>)(CO<sub>3</sub>)<sub>3</sub> mon/C2/c

SERIES K LINEKITE, orth/Pnnm. Structure not known. Plášil, J., Fejfarová, K., Sejkora, J., Čejka, J., Novák, M., Škoda,

R., Hloušek, J., Dušek, M. and Cĺsařová, I. (2013) Línekite, IMA 2012-066. CNMNC Newsletter No. 15, February

2013, page 7; Mineralogical Magazine, 77, 1-12.

JECKA LINEKITE  $K_2Ca_3[(UO_2)(CO_3)_3]_2.7H_2O$ 

SERIES L BRAUNERITE, mon/P2<sub>1</sub>/c.

JECLA BRAUNERITE K<sub>2</sub>Ca(UO<sub>2</sub>)(CO<sub>3</sub>)<sub>3</sub>.6H2O

**SERIES M** 

LEOSZILARDITE, mon/C2/m. The structure of leószilárdite is unique amongst the uranyl carbonates with respect to the arrangement of Na+ and Mg2+ cations, and represents the first natural uranyl carbonate containing both Na and Mg as essential constituents. The uranyl hexagonal bipyramid shares two edges with face-sharing chains of Na(H2O)O₅ trigonal prisms (Na2) that extend along [010].The structure also contains a distinctive three-octahedron unit of the formula Na2MgO12(H2O)4 consisting of two Na-centered octahedra that share the opposite faces of a Mgcentered octahedron at the center (Na1-Mg1-Na1).

These three-octahedron units, aligned along [101], further connect the UTC units. Chains of Nacentered polyhedra found in čejkaite coordinate to UTCunits by sharing only apices with carbonate triangles from six individual uranyl polyhedra. In contrast, each Na-centered polyhedron in the chains of ježekite shares one edge with a uranyl polyhedron and one apex with the carbonate triangle of a different UTC unit. Individual Na-centered octahedra in the chains of leószilárdite coordinate to three UTC units, sharing two edges of uranyl polyhedra and one apex of a CO<sub>3</sub> triangle,

JECMA LEOSZILARDITE Na<sub>6</sub>Mg(UO<sub>2</sub>)<sub>2</sub>(CO<sub>3</sub>)<sub>6</sub>.6H<sub>2</sub>O

**SERIES N** 

MARKEYITE, orth/Pmmn. The new mineral markeyite (IMA2016-090), Ca9(UO2)4(CO3)13-28H2O, was found in the Markey mine, San Juan County, Utah, USA, where it occurs as a secondary phase on asphaltum in association with calcite, gypsum and natrozippeite. The mineral is pale yellowish-green with white streak and fluoresces bright bluish white under a 405 nm laser. Crystals are transparent and have vitreous to pearly lustre. It is brittle, with Mohs hardness 11/2 to 2, irregular fracture and three cleavages: perfect on {001}; good on {100} and {010}. The measured density is 2.68 g cm-3. Crystals are blades, flattened on {001} and elongate on [010], exhibiting the forms {100}, {010}, {001}, {110}, {101}, {011} and {111}. Markeyite is optically biaxial (–) with  $\alpha = 1.538(2)$ ,  $\beta = 1.542(2)$  and  $\gamma = 1.538(2)$ 1.545(2) (white light); the measured 2V is 81(2)°; the dispersion is r < v (weak); the optical orientation is X = c, Y = b, Z = a; and pleochroism is X = light greenish yellow, Y and Z = light yellow (X > Y  $\approx$  Z). Electron microprobe analyses (energy-dispersive spectroscopy mode) yielded CaO 18.60, UO3 42.90, CO2 21.30 (calc.) and H2O 18.78 (calc.), total 101.58 wt.% and the empirical formula Ca8.91(U1.01O2)4(CO3)13 28H2O. The six strongest powder X-ray diffraction lines are [dobs Å(I)(hkl)]: 10.12(69)(001), 6.41(91)(220,121), 5.43(100)(221), 5.07(33)(301,002,131), 4.104(37)(401,141) and 3.984(34)(222). Markeyite is orthorhombic, Pmmn, a = 17.9688(13), b = 18.4705(6), c = 10.1136(4) Å, V = 3356.6(3) Å3 and Z = 2. The structure of markeyite (R1 = 0.0435 for 3427 Fo  $> 4\sigma F$ ) contains uranyl tricarbonate clusters (UTC) that are linked by Ca-O polyhedra forming thick corrugated heteropolyhedral layers. Included within the layers is an additional disordered CO3 group linking the Ca-O polyhedra. The layers are linked to one another and to interlayer H2O groups only via . The structure bears some similarities to that of liebigite.

 JECNA
 MARKEYITE
  $Ca_9(UO_2)_4(CO_3)_{13}.28H_2O$  

 JECNB
 PSEUDOMARKEYITE
  $Ca_8(UO_2)_4(CO_3)_{12}.21H_2O$  

 JECNC
 NATROMARKEYITE
  $Na_2Ca_8(UO_2)_4(CO_3)_{13}.27H_2O$ 

SERIES O PADDLEWHEELITE, mon/Pc. MgCa5Cu2[(UO2)(CO3)3]4-33H2O, is a new uranyl carbonate mineral found underground in the Svornost mine, Jáchymov District, Bohemia, Czech

Republic, where it occurs as a secondary oxidation product of uraninite. The conditions leading to its crystallization are complex, likely requiring concomitant dissolution of uraninite, calcite, dolomite, chalcopyrite, and andersonite. Paddlewheelite is named after its distinctive structure, which consists of paddle-wheel clusters of uranyl tricarbonate units bound by square pyramidal copper "axles" and a cubic calcium cation "gearbox." Paddle wheels share edges with calcium polyhedra to form open sheets that are held together solely by hydrogen bonding interactions. The new mineral is monoclinic, Pc, a = 22.052(4), b = 17.118(3), c = 19.354(3) Å, beta = 90.474(2), V = 7306(2) Å3 and Z = 4. Paddlewheelite is the second-most structurally complex uranyl carbonate mineral known after ewingite and its structure may provide insights into the insufficiently described mineral voglite, as well as Cu-U-CO3 equilibrium in general.

JECOA PADDLEWHEELITE

 $MgCa_5Cu_2(UO_2)_4(CO_3)_{12}(H_2O)_{33}$ 

TYPE D URANYL CARBONATES WITH UO<sub>2</sub>: CO<sub>3</sub> = 1:4

SERIES A VOGLITE, mon/P2<sub>1</sub> or P2<sub>1</sub>/m. Structure not known. Vogl (1853) Geol. Reichsanst. Jahrb., Vienna: 4: 222-223 (as Uran-Kalk-Kupfer-Carbonat).

Haidinger (1853) Geol. Reichsanst. Jahrb., Vienna: 4: 223.

Schrauf (1873) Mineralogische und petrographische Mitteilungen, Vienna: 138.

Larsen, E.S. (1921) The Microscopic Determination of the Nonopaque Minerals, First edition, USGS Bulletin 679: 154.

Palache, C., Berman, H., & Frondel, C. (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: 237.

Journal of the Czech Geological Society, Prague (1997): 42: 453-455.

JEDAA VOGLITE  $Ca_2Cu(UO_2)(CO_3)_4 \cdot 6H_2O$  mon/P2<sub>1</sub>/m

SERIES B

SHABAITE, mon/P2.m, Pm or P2. Structure contains two independent U, two Ca, four Nd, seven C and 48 O sites. Both of the U atoms are surrounded by eight O atoms forming hexagonal uranyl bipyramids, chelated by carbonate groups to form the well-known uranyltricarbonate clusters. The symmetrically related Nd atoms form infinite chains by sharing common edge of the polyhedra. These chains extend // to c. Adjacent chains are linked through the carbonate groups to form Nd-(H<sub>2</sub>O-CO<sub>3</sub> sheets that are stacked perpendicular to b. Between these sheets the UTC and Capolyhedra are located. Adjacent sheets are linked to the interstitial complex via carbonate groups, staggered towards the interlayer, and by the H-bonds. European Journal of Mineralogy (1989): 1: 85-88.

The structure of shabaite-(Nb) is based upon finite clusters of polyhedra, the well-known uranyl-tricarbonate cluster, the Ca-polyhedra linked to UTC and infinite sheets of Nb0-polyhedra with internal Nd-O-C linkages. The infinite sheets of Nd-polyhedra are stacked perpendicular to c; fo9rming electroneutral layers. Adjacent layers are linked by H bonds. Journal of Geosciences, 62, 97-105.

American Mineralogist (1990): 75: 433-434.

 $\label{eq:lemma:lemma:shabalte-(Nd)} \mbox{ $Ca(Nd,Sm,Y)_2(UO_2)(CO_3)_4(OH)_2$:$6H_2O$ $mon/P2_1,Pm,P2/m$}$ 

SERIES C ASTROCYANITE, hex/P6/mmm. Structure not known. New Minerals (1997), New Minerals 1990-1994.

European Journal of Mineralogy (1990): 2: 407-411.

JEDCA ASTROCYANITE-(Ce) Cu<sub>2</sub>Ce<sub>2</sub>(UO<sub>2</sub>)(CO<sub>3</sub>)<sub>5</sub>(OH)<sub>2</sub>·0.5H<sub>2</sub>O hex/P6mmm

TYPE E URANYL CARBONATES WITH UO<sub>2</sub>:CO<sub>3</sub> = 1:5

SERIES A URANCALCARITE, orth/Pbnm or Pbn2<sub>1</sub>. Structure unknown. Bulletin de la Société française de Minéralogie et de Cristallographie (1984): 107: 21-24.

American Mineralogist (1985): 70: 438-439.

JEEAA URANCALCARITE Ca(UO<sub>2</sub>)<sub>3</sub>(CO<sub>3</sub>)(OH)<sub>6</sub>·3H<sub>2</sub>O

SERIES B WYARTITE, orth/P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>. The structure consists of three unique U positions; two containing U<sup>6+</sup> and

involve uranyl ions with typical pentagonal-bypyramidal coordinations. The U $\Phi_7$  polyhedra share edges and corners to form a unique sheet in which a CO<sub>3</sub> group shares an edge with the U $^{5+}\Phi_7$  polyhedron. The Ca $\Phi_7$  polyhedron is linked to one adjacent sheet by sharing an edge with the carbonate group and an O atom with the U polyhedron. Structure consists of U $^{6+}$  in dipyramidal U $^{[2+5]}$  coordination forming chains // [001] by sharing edges of the dipyramids; these are connected by sharing edges with U $^{5+}$  polyhedra, UO<sub>4</sub>(OH)O(H<sub>2</sub>O), to build sheets // (001). Appended to the sheets are CO<sub>2</sub>OH triangles and Ca polyhedra; the sheets are linked by H-bonding from water molecules

JEEBA WYARTITE Ca<sub>3</sub>U<sup>5+</sup>(UO<sub>2</sub>)<sub>2</sub>(CO<sub>3</sub>)O<sub>4</sub>(OH)(H<sub>2</sub>O)<sub>7</sub>

SERIES C ROUBAULTITE, tric/P1. . Structure consists of rutile-like chains // [010] composed of edge-sharing

CuO₂(OH)₂(H₂O)₂ octahedra, and chains of edge-sharing UO(OH)O₅ and UO₂O⁶ polyhedra, also //

[010], are connected into sheets // (101) by sharing carbonate groups.

JEECA ROUBAULTITE  $Cu_2(UO_2)_3O_2(CO_3)_2(OH)_2$ :4 $H_2O$  tric/P1 or P1

SERIES D open

SERIES E SHARPITE, orth. Structure not known. Mélon (1938) Bull. séan. inst. roy. colon. Belge 9: 333.

American Mineralogist (1939): 24: 658.

Palache, C., Berman, H., & Frondel, C. (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: 275.

American Mineralogist (1985): 70: 220.

JEEEA SHARPITE Ca(UO<sub>2</sub>)<sub>6</sub>(CO<sub>3</sub>)<sub>5</sub>(OH)<sub>4</sub>·6H<sub>2</sub>O

TYPE F URANYL CARBONATES WITH UO<sub>2</sub>: CO<sub>3</sub> = 2:1

SERIES A OSWALDPEETERSITE, mon/P2<sub>1</sub>/c. Structure not known. Canadian Mineralogist (2001): 39: 1685-1689.

JEFAA OSWALDPEETERSITE (UO<sub>2</sub>)<sub>2</sub>(CO<sub>3</sub>)(OH)<sub>2</sub>·4H<sub>2</sub>O

TYPE G URANYL CARBONATES WITH SULFATE, SILICATE OR PHOSPHATE

SERIES A SCHROECKINGERITE, orth/Cmmm. Pseudo-hexagonal [001]; sheets // (001) are formed by three

CaFO<sub>5</sub>(H<sub>2</sub>O)<sub>2</sub> polyhedra, one NaO<sub>3</sub>(H<sub>2</sub>O)<sub>3</sub> octahedron, one uranyl-carbonate unit and jone Ca-bonded sulphate tetrahedron; four free water molecules are accommodated between the sheets, with only H-

bonding between sheets.

JEGAA SCHROECKINGERITE NaCa<sub>3</sub>(UO<sub>2</sub>)(CO<sub>3</sub>)<sub>3</sub>(SO<sub>4</sub>)F<sup>-</sup>10H<sub>2</sub>O

SERIES B NASLEDOVITE, Structure not known. American Mineralogist (1959): 44: 1325.

JEGBA NASLEDOVITE Q/D PbMn<sub>3</sub>Al<sub>4</sub>(CO<sub>3</sub>)<sub>4</sub>(SO<sub>4</sub>)O<sub>5</sub>·5H<sub>2</sub>O

SERIES C LEPERSONNITE, orth/Pnnm or Pnn2. Structure not known. American Mineralogist (1983): 68: 1248

JEGCA LEPERSONNITE-(Gd)  $Ca(Gd,Dy)_2[(UO_2)_6/O_3/(CO_3)_2/SiO_4]_4$  60H<sub>2</sub>O

GROUP F SPECIAL PHASES CONTAINING CARBONATE + OTHER ANIONIC GROUPS

TYPE A POLYOXOMETALATE CLUSTERS

SERIES A RAMAZZOITE, cubic/P43m. Structure contains the first polyoxometalate cluster known.

Ramazzoite Q1 (IMA2017-090), [Mg8Cu12(PO4)(CO3)4(OH)24(H2O)20][(H0.33SO4)3(H2O)36], is a new polyoxometalate (POM) mineral from the Monte Ramazzo mine, near Genova, Liguria, Italy. It occurs on magnetite-rich matrix in association with chlorartinite, chrysotile, dypingite, goethite, lepidocrocite and nesquehonite, and is a late-stage, secondary mineral crystallizing from low-temperature, aqueous solutions. Ramazzoite forms as simple cubes up to about 0.15mm on edge. The mineral is blue to greenish-blue with a vitreous to oily lustre and pale blue streak. Crystals are very brittle with conchoidal fracture, and a perfect cleavage on  $\{100\}$ . The Mohs' hardness is  $2\frac{1}{2}$ . The measured density is 1.98(1) g cm-3. The mineral is soluble with mild effervescence in dilute HCl at room temperature. Optically, ramazzoite is isotropic with n = 1.491(1) (white light). Electron microprobe analyses (with CO2 from structural data and H2O from density) gave the empirical formula [(Mg8.00)(Cu8.00Mg3.78)(PO4)(CO3)4(OH)24(H2O)20] [(H0.65S1.01O4)3(H2O)36], based on 1 P atom per formula unit (apfu). Ramazzoite is cubic, P-43m, with the unit-cell parameters: a = 13.3887(10)Å, V = 2400.0(5)Å3 and Z = 1. The crystal structure, refined to R1 = 0.064 for 803 observed reflections [I >  $2\sigma$ I], contains a novel [Mg8Cu12(PO4)(CO3)4(OH)24(H2O)20]5+ POM cation.

JFAAA RAMAZZOITE  $[Mg_8Cu_{12}(PO_4)(CO_3)_4(OH)_{24}(H_2O)_{20}][(H_{0.33}SO_4)_3(H_2O)_{36}]$ 

Updated 05/20/19