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McCRILLISITE, $NaCs(Be,Li)Zr_2(PO_4)_4 \cdot 1–2H_2O$, A NEW MINERAL SPECIES FROM MOUNT MICA, OXFORD COUNTY, MAINE, AND NEW DATA FOR GAINESITE

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ABSTRACT

Mccrillisite, ideally $NaCs(Be,Li)Zr_2(PO_4)_4 \cdot 1–2H_2O$, a member of the gainesite group, occurs in the Mount Mica granitic pegmatite, South Paris, Oxford County, Maine. The mineral is a product of late-stage hydrothermal alteration and is associated with approximately twenty other silicate, oxide, carbonate, arsenide and phosphate minerals. Crystals occur in mm- to cm-sized cavities, and individuals are up to 1.2 mm in maximum dimension. The crystals are white to colorless, bipyramidal, with {111} dominant and {001} minor. Streak is white, and luster, vitreous; the mineral is translucent to transparent, and nonfluorescent. Hardness (Mohs) is 4 to 4½. No cleavage was observed, and the fracture is conchoidal. $D_{measured}$ 3.125(5), $D_{calculated}$ 3.30 g/cm^3. Mccrillisite is uniaxial positive, with ω 1.634(2) and ε 1.645(2), colorless and nonpleochroic. The mineral is tetragonal, $I4_1/amd$, with a 6.573(2), c 17.28(2) Å, V 746.6(9) Å^3, c/a 2.6289, Z = 2. The strongest six reflections in the X-ray powder-diffraction pattern [d(Å)(I)(hkl)] are: 6.159(90)(101), 4.326(80)(004), 4.099(40)(112), 3.281(80)(200), 3.060(100)(105) and 2.896(30)(211). Chemical compositions (wt.%) for mccrillisite and cotype gainesite, respectively, are: Li_2O 0.6, 0.8; Al_2O_3 <0.1, 0.5; CaO <0.1, 0.7; MgO 0.1, 0.35; MnO <0.1, 0.7; FeO <0.1, 1.0; SrO 0.2, – –; Na_2O 4.2, 7.8; K_2O 0.3, 2.4; Cs_2O 15.3, 2.2; BeO 2.9, 2.3; ZnO 0.5, <0.1; ZrO_2 31.6, 33.0; HfO_2 2.5, 0.7; P_2O_5 38.3, 45.0; Rb_2O <0.1, 0.1; F 0.5, <0.1; H_2O 3.0, 4.3; subtotal 100.10, 101.95; O = F 0.21, – –; total 99.89, 101.95. An empirical formula for mccrillisite, based on 4 P atoms, is: $Na_{1.00}(Cs_{0.80}Li_{0.18}K_{0.05})_{\Sigma 1.03}(Be_{0.86}Li_{0.12}Mg_{0.02})_{\Sigma 1.00}(Zr_{1.90}Hf_{0.09}Zn_{0.05})_{\Sigma 2.04}(P_{4.00}Si_{0.01})_{\Sigma 4.01}(O_{15.8}F_{0.2})_{\Sigma 16.0} \cdot 1.23H_2O$. The empirical formula for gainesite, based on 4 P atoms, is: $Na_{1.00}(Na_{0.59}K_{0.32}Cs_{0.10}Rb_{0.01})_{\Sigma 1.02}(Be_{0.58}Li_{0.34}Mg_{0.06}Al_{0.06})_{\Sigma 10.4}(Zr_{1.69}Fe_{0.09}Ca_{0.08}Mn_{0.06}Hf_{0.02})_{\Sigma 1.94}(P_{4.00}Si_{0.01})_{\Sigma 4.01}O_{15.6} \cdot 1.5H_2O$. Gainesite was originally considered to be anhydrous, but is shown to contain essential molecular water, as does mccrillisite. The mineral name honors the McCrillis family, particularly the late Dean McCrillis and Philip McCrillis, of Oxford County, Maine, and their more than 90 years spent working the granitic pegmatites of Maine.

Keywords: mccrillisite, new mineral species, Na, Cs, Be, Zr phosphate, gainesite, granitic pegmatite, Mount Mica, Oxford County, Maine.

SOMMAIRE

La mccrillisite, membre nouvellement découvert du groupe de la gainesite ayant la formule chimique idéale $NaCs(Be,Li)Zr_2(PO_4)_4 \cdot 1–2H_2O$, provient de la pegmatite granitique de Mount Mica, à South Paris, comté d'Oxford, au Maine. Il s'agit d'un produit d'une altération hydrothermale tardive, associé à une vingtaine d'autres silicates, oxydes, carbonates, arséniures et phosphates. Les cristaux se trouvent dans des cavités millimétriques à centimétriques, et ont une longueur maximale de 1.2 mm. Les cristaux sont blancs ou incolores, bipyramidaux, avec {111} dominant et {001} de moindre importance. La rayure est blanche, et l'éclat, vitreux; les cristaux sont translucides à transparents, et non fluorescents. La dureté de Mohs est entre 4 et 4½. La densité mesurée est 3.125, et la densité calculée, 3.30. La mccrillisite est uniaxe positive, avec ω 1.634(2) et ε 1.645(2), incolore et non pléochroïque. C'est un minéral tétragonal, $I4_1/amd$, avec a 6.573(2), c 17.28(2) Å, V 746.6(9) Å^3,

c/a 2.6289, $Z = 2$. Les six raies les plus intenses du spectre de diffraction (méthode des poudres) [*d*(Å)(I)(*hkl*)] sont: 6.159(90)(101), 4.326(80)(004), 4.099(40)(112), 3.281(80)(200), 3.060(100)(105) et 2.896(30)(211). La composition chimique de la mccrillisite et de la gainesite cotype (en %, poids) est: Li_2O 0.6, 0.8; Al_2O_3 <0.1, 0.5; CaO <0.1, 0.7; MgO 0.1, 0.35; MnO <0.1, 0.7; FeO <0.1, 1.0; SrO 0.2, – –; Na_2O 4.2, 7.8; K_2O 0.3, 2.4; Cs_2O 15.3, 2.2; BeO 2.9, 2.3; ZnO 0.5, <0.1; ZrO_2 31.6, 33.0; HfO_2 2.5, 0.7; P_2O_5 38.3, 45.0; Rb_2O <0.1, 0.1; F 0.5, <0.1; H_2O 3.0, 4.3; sous-total 100.10, 101.95; O = F 0.21, – –; total 99.89, 101.95. La formule empirique de la mccrillisite, sur une base de 4 atomes de P, est: $Na_{1.00}(Cs_{0.80}Li_{0.18}K_{0.05})_{\Sigma 1.03}(Be_{0.86}Li_{0.12}Mg_{0.02})_{\Sigma 1.00}(Zr_{1.90}Hf_{0.09}Zn_{0.05})_{\Sigma 2.04}(P_{4.00}Si_{0.01})_{\Sigma 4.01}(O_{15.8}F_{0.2})_{\Sigma 16.0}\cdot 1.23H_2O$. La formule empirique de la gainesite, aussi pour 4 atomes de P, est: $Na_{1.00}(Na_{0.59}K_{0.32}Cs_{0.10}Rb_{0.01})_{\Sigma 1.02}(Be_{0.58}Li_{0.34}Mg_{0.06}Al_{0.06})_{\Sigma 10.4}(Zr_{1.69}Fe_{0.09}Ca_{0.08}Mn_{0.06}Hf_{0.02})_{\Sigma 1.94}(P_{4.00}Si_{0.01})_{\Sigma 4.01}O_{15.6}\cdot 1.5H_2O$. On croyait la gainesite anhydre, mais elle contient de l'eau moléculaire, tout comme la mccrillisite. Le nom honore la famille McCrillis, et particulièrement feu Dean McCrillis et Philip McCrillis, du comté d'Oxford, pour quatre-vingt-dix années d'éxploitation des pegmatites granitiques du Maine.

(Traduit par la Rédaction)

Mots-clés: mccrillisite, nouvelle espèce minérale, phosphate de Na, Cs, Be, et Zr, gainesite, pegmatite granitique, Mount Mica, comté d'Oxford, Maine.

INTRODUCTION

A rock specimen containing a doubly terminated crystal suspected to be gainesite, approximately 1.2 mm long, and two smaller crystals, was sent in 1991 by Vandall T. King of Rochester, New York to one of us (EEF) for identification. The specimen was collected in the Mount Mica granitic pegmatite, South Paris, Oxford County, Maine in 1989 by Mr. Gene T. Bearss of Sanford, Maine. The mineral, which turned out to be a new species, mccrillisite, occurred in a boulder, approximately 1 × 1.2 × 1.6 m, which was originally mined in 1977–1978, subsequently bulldozed, and then re-exposed in 1988. Associated minerals (identified by X-ray diffraction, optical properties, and scanning electron microscropy – energy dispersion spectroscopy methods) are: albite, quartz, manganoan almandine, muscovite, siderite, fluorapatite, elbaite, lepidolite, beryl, montebrasite, rhodochrosite, cassiterite, manganocolumbite, uraninite, löllingite, zircon, eosphorite, moraesite, iron-rich roscherite and kosnarite (Brownfield *et al.* 1993, Tealdi 1993). The mineral occurs in open cavities up to several centimeters across and is very late in the paragenesis. It formed as a result of late-stage hydrothermal alteration of earlier-formed Zr-bearing minerals in the pegmatite, as evidenced by the presence of corroded zircon. Both kosnarite and this new mineral species occur in cavities within blue tourmaline "eyes", as described by King (1992). X-ray powder-diffraction studies show a gainesite-type pattern, but with the diffraction lines slightly displaced from those published for gainesite. SEM–EDS analysis showed substantial Cs, and the existence of a Cs-analog was immediately suspected.

The mineral is named *mccrillisite* in honor of the McCrillis family, particularly the late Dean McCrillis and his son, Philip McCrillis, of Oxford County, Maine, for their more than 90 years spent working the granitic pegmatites of Maine. The mineral and the name have been approved in advance of publication, by the Commission on New Minerals and Mineral Names, IMA. Holotype material (catalogue number NMNH 170853) has been deposited at the U.S. National Museum (Smithsonian Institution).

INSTRUMENTATION

Electron-microprobe analyses were made with an ARL SEMQ instrument at an operating voltage of 15 kV, and 10 nA sample current, and a beam diameter of 5 μm. Counting times were 20 or 40 seconds on peak positions and 10 seconds on background positions. Standards utilized were: natural pollucite (Rb, Cs), synthetic RbCl (Rb), natural albite (Na), natural orthoclase (K), natural apatite (P), synthetic zircon and ZrO_2 (Zr), synthetic Hf metal (Hf), synthetic CaF_2 (F), natural pyrope (Al, Si, Fe, and Mg), and natural manganoan willemite (Mn). Data reduction was carried out using a modified version of MAGIC IV. Ion-microprobe analyses were made on an A.E.I. IM20 instrument (University of Chicago). Laser-ablation (LA) inductively coupled plasma – mass spectrometry (ICP–MS) analyses were made using a Fisons VG PlasmaQuad 2+ instrument equipped with a Nd/YAG laser operated at 1064 nm. X-ray powder-diffraction studies were carried out using 114.6-mm-diameter Gandolfi cameras. X-ray single-crystal studies were done using Huber precession cameras utilizing Zr-filtered Mo radiation. Density was determined on multiple, optically pure, mineral fragments using sink–float techniques in a methylene iodide – acetone mixture.

PHYSICAL PROPERTIES

Crystals of mccrillisite are white to colorless, translucent to transparent, and occur as bipyramidal crystals as much as 1.2 mm in maximum dimension. The dominant form is {111}, and the minor form is {001}. A color photograph of the mineral is shown in Tealdi (1993). Only about seven matrix specimens are

known; the total weight of all of the crystals is about 8 mg. The streak is white, and the luster, vitreous; it is nonfluorescent and nonluminescent; no cleavage was observed. The fracture is conchoidal, the hardness (Mohs), 4 to 4½, the specific gravity, 3.125(5), and D(calc.) for the empirical formula is 3.30 g/cm^3. Many crystals have a characteristic "crackled" appearance, which may be due to partial dehydration.

Crystallography and X-Ray-Diffraction Data

Precession camera studies show that mccrillisite is tetragonal, $I4_1/amd$, with unit-cell parameters refined from powder data: a 6.573(2), c 17.28(2) Å, V 746.6(9) Å^3, c/a 2.6289, Z = 2. No twinning was observed on precession films. Indexed X-ray powder-diffraction data are given in Table 1. Comparison of unit cell, optical, and density data for all three members of the gainesite group are given in Table 2.

TABLE 1. X-RAY POWDER-DIFFRACTION DATA FOR McCRILLISITE

I/I$_o$	d(meas.)Å	d(calc.)Å	hkl
90	6.159	6.144	101
80	4.326	4.320	004
40	4.099	4.093	112
80	3.281	3.287	200
100	3.060	3.059	105
30	2.896	2.898	211
20	2.616	2.616	204
20	2.316	2.311	107
15	2.239	2.239	215
10	2.172	2.174	301
5	2.050	2.048	303
25	2.017	2.021	312
30	1.849	1.850	305
20	1.811	1.813	321
3	1.745	1.744	306
15	1.687	1.685	316
5	1.644	1.643	400
10	1.617	1.614	402
5	1.589	1.587	411
15	1.526	1.525	322
10	1.470	1.470	420
10	1.446	1.448	415
3	1.390	1.391	424
8	1.367	1.364	336
15	1.331	1.329	31$\underline{1}$0
8	1.313	1.311	431

Additional reflections to 0.7935 Å are present. The data were collected using a 114.6-mm diameter Gandolfi camera with natural corundum as an internal standard. CuKα (Ni-filtered) radiation (λ = 1.54178 Å). The intensities were estimated visually.

TABLE 2. COMPARISON OF DATA ON UNIT CELL, OPTICAL PROPERTIES, DENSITY, AND ALKALI-SITE OCCUPANCY FOR MEMBERS OF THE GAINESITE GROUP

	Gainesite	Selwynite	Mccrillisite
Unit-cell parameters			
a(Å)	6.567	6.570	6.573
c(Å)	17.119	17.142	17.28
V(Å^3)	738.35	739.9	746.6
Optical data	uniaxial (+)	uniaxial (+)	uniaxial (+)
ω	1.618	1.624	1.634
ε	1.630	1.636	1.645
birefringence	0.12	0.12	0.11
Density			
measured	2.94	2.94	3.125
calculated (g/cm^3)	2.89	3.07	3.30
Alkali site occupancy	NaNa	NaK	NaCs

Data for gainesite from Moore *et al.* (1983). Data for selwynite from W.D. Birch (pers. comm., 1993). Data for mccrillisite from this study.

Chemistry

A combination of electron microprobe, LA–ICP–MS, and ion-microprobe analytical methods were used to determine the chemical composition of mccrillisite and cotype gainesite (provided by the USNM). Proportions of ZnO, BeO, and Li_2O were determined by LA–ICP–MS and ion microprobe. Hydrogen (expressed as water) was determined by ion microprobe. The chemical composition of the two minerals is given in Table 3.

Empirical formulas (on the basis of 4 P atoms) for mccrillisite and gainesite, respectively, are: $Na_{1.00}(Cs_{0.80}Li_{0.18}K_{0.05})_{\Sigma 1.03}(Be_{0.86}Li_{0.12}Mg_{0.02})_{\Sigma 1.00}(Zr_{1.90}Hf_{0.09}Zn_{0.05})_{\Sigma 2.04}(P_{4.00}Si_{0.01})_{\Sigma 4.01}(O_{15.8}F_{0.2})_{\Sigma 16.0}\cdot 1.23H_2O$ and $Na_{1.00}(Na_{0.59}K_{0.32}Cs_{0.10}Rb_{0.01})_{\Sigma 1.02}(Be_{0.58}Li_{0.34}Mg_{0.06}Al_{0.06})_{\Sigma 1.04}(Zr_{1.69}Fe_{0.09}Ca_{0.08}Mn_{0.06}Hf_{0.02})_{\Sigma 1.94}(P_{4.00}Si_{0.01})_{\Sigma 4.01}O_{15.6}\cdot 1.5H_2O$.

Optical Data

Mccrillisite is uniaxial positive, with ω equal to 1.634(2) and ε 1.645(2), as measured in blue-filtered white light. Some grains are anomalously biaxial, with $2V$ to 5°. Using the observed density of 3.125 g/cm^3, the Gladstone–Dale compatibility index, $1-(K_P/K_C)$, is –0.094 and is thus categorized as poor. Possible reasons for this are a low measured density or imperfectly known molar refractivities, or both. If the calculated density of 3.30 g/cm^3 is used, the compatibility index is –0.036 (excellent). Similar calculations for gainesite, using the chemical data presented in Table 3, result in compatibility indices of –0.057 (with

TABLE 3. CHEMICAL COMPOSITION OF MEMBERS OF THE GAINESITE GROUP

	Mccrillisite	Gainesite	Gainesite*	Selwynite
Li_2O	0.6	0.8	1.7	—
Al_2O_3	<0.1.	0.5	1.21	1.04
BeO	2.9	2.3	2.8	1.43
Na_2O	4.2	7.8	6.81	4.77
MgO	0.1	0.35	0.30	0.15
P_2O_5	38.3	45.0	45.0	40.90
K_2O	0.3	2.4	1.45	6.26
CaO	<0.1	0.7	0.86	0.98
MnO	<0.1	0.7	0.83	0.99
FeO	<0.1	1.0	0.54	0.49
SrO	0.2	0.0	0.15	0.16
ZnO	0.5	<0.1	4.11	—
SiO_2	0.1	0.1	0.59	0.49
Rb_2O	<0.1	0.1	0.11	0.20
ZrO_2	31.6	33.0	33.0	33.76
Cs_2O	15.3	2.2	1.93	0.70
HfO_2	2.5	0.7	—	1.17
H_2O	3.0	4.3	—	5.40
F	0.5	<0.1	—	0.37
Subtotal	100.10	101.95	101.39	99.45
O=F	0.21	0.0	0.0	0.16
Total	99.89	101.95	101.39	99.29

All values are given in weight percent.
Selwynite also contains 0.16 wt. % BaO and 0.03 wt. % Ce_2O_3.
Analyses of mccrillisite and gainesite are averages of five analyses each (this study).
* - from Moore et al. 1983.
Analysis of selwynite is from W.D. Birch (pers. comm., 1993).

calculated density of 2.89 g/cm^3) and –0.040 (with measured density of 2.94 g/cm^3); these compatibility values are good, according to the ranking of Mandarino (1979, 1981).

Discussion and Conclusions

The gainesite group of minerals is now known to contain three members: gainesite, mccrillisite and selwynite (Birch *et al.* 1995). Only four other naturally occurring Zr phosphates are known: kosnarite, $KZr_2(PO_4)_3$, mahlmoodite, $FeZr(PO_4)_2{\cdot}4H_2O$ (Milton *et al.* 1993), voggite, $Na_2Zr(PO_4)(CO_3)(OH){\cdot}H_2O$, and wycheproofite, $NaAlZr(PO_4)_2(OH)_2{\cdot}H_2O$ (Birch *et al.* 1995). It is now clear that all three members of the gainesite group are hydrated, containing between 1 and 2 molecules of water. In contradiction to what was previously reported (Moore *et al.* 1983), gainesite contains no Zn. One of the crystals used by Moore for his single-crystal studies was chemically analyzed by us and found to contain no Zn. The lavender to deep purple colors of gainesite and selwynite, respectively, are due to Mn (presumably small amounts of Mn^{3+} or Mn^{4+}, or both) substituting for Zr. Mccrillisite is colorless to white and contains no Mn. It is also clear that two alkali sites, one large and the other small, exist in the structure, as previously proposed by Moore *et al.* (1983). Na is dominant in the smaller site of all three minerals, whereas Na, K, Cs, or presumably Rb, predominate in the large site. An Rb-dominant member thus could be found in the future. Because of the small grain-size, occurrences of members of the gainesite group are probably more numerous than presently known.

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