Canadian Mineralogist
Vol. 24, pp. 599-604 (1986)

BOBFERGUSONITE: A NEW PRIMARY PHOSPHATE MINERAL FROM CROSS LAKE, MANITOBA

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ABSTRACT

The new mineral species bobfergusonite occurs as abundant, large anhedral crystals in a granitic pegmatite at Cross Lake, Manitoba. It ranges in color from red-brown (holotype) to green-brown, has a yellow-brown streak, resinous lustre and is nonfluorescent. The measured density is 3.54(1) g/cm³; the hardness is 4. It is biaxial (+), α 1.694(1), β 1.698(1), γ 1.715(2), $2V$ 46.4(2)°, pleochroism $X = Y$ yellow-orange, Z orange, $Y \parallel b$ and $a \wedge X = +10°$ in the β angle. The average chemical composition for the holotype (wt.%) is: Na_2O 6.8, MgO 0.3, CaO 1.2, MnO 31.7, FeO 0.3, ZnO 0.1, Al_2O_3 7.5, Fe_2O_3 6.9, P_2O_5 45.2, H_2O 0.3, total 100.3. The semiempirical formula, $(Na_{2.07}Mn_{0.53}Ca_{0.20}\square_{1.20})_{\Sigma 4}(Mn_{3.68}Al_{1.39}Fe^{3+}_{0.81}Mg_{0.07}Fe^{2+}_{0.04}Zn_{0.01})_{\Sigma 6}P_{5.99}(O_{23.69}OH_{0.31})_{\Sigma 24}$ considered with structural data, gives the ideal formula $Na_2Mn_5Fe^{3+}Al(PO_4)_6$ ($Z = 4$). The six strongest lines of the X-ray powder pattern [d in Å, $I > 40$] are 3.05(100), 2.87(66), 2.71(49), 2.51(53), 2.08(67) and 1.58(43). The unit-cell parameters are a 12.773(2), b 12.486(2), c 11.038(2) Å, β 97.15°; the space group is $P2_1/n$. It is most closely related to wyllieite-group minerals, from which it differs in both structure and composition. The mineral is named after Dr. Robert Bury Ferguson.

Keywords: bobfergusonite, new mineral, phosphate, granitic pegmatite, Manitoba, wyllieite, alluaudite.

SOMMAIRE

La bobfergusonite, nouvelle espèce minérale, forme de larges cristaux idiomorphes en abondance dans la pegmatite granitique du lac Cross, au Manitoba. Sa couleur va du rouge-brun (holotype) au vert-brun; sa rayure est jaune-brun, et son éclat, résineux. Elle n'est pas fluorescente. Densité mesurée 3.54(1), dureté 4. Elle est biaxe positive, α 1.694(1), β 1.698(1), γ 1.715(2), $2V$ 46.4(2)°, pléochroïsme $X = Y$ jaune-orange, Z orange, $Y \parallel b$, $a \wedge X = +10°$ dans l'angle β. Sa composition moyenne (% en poids) d'après les résultats analytiques sur l'échantillon holotype, est: Na_2O 6.8, MgO 0.3, CaO 1.2, MnO 31.7, FeO 0.3, ZnO 0.1, Al_2O_3 7.5, Fe_2O_3 6.9, P_2O_5 45.2, H_2O 0.3, total 100.3. La formule semi-empirique, $(Na_{2.07}Mn_{0.53}Ca_{0.20}\square_{1.20})_{\Sigma 4}(Mn_{3.68}Al_{1.39}Fe^{3+}_{0.81}Mg_{0.07}Fe^{2+}_{0.04}Zn_{0.01})_{\Sigma 6}P_{5.99}(O_{23.69}OH_{0.31})_{\Sigma 24}$ considérée à la lumière des données structurales, mène à la formule idéalisée $Na_2Mn_5Fe^{3+}Al(PO_4)_6$ ($Z = 4$). Les six raies les plus intenses du cliché de poudre [d in Å, $I > 40$] sont: 3.05(100), 2.87(66), 2.71(49), 2.51(53), 2.08(67) et 1.58(43). Les paramètres réticulaires sont: a 12.773(2), b 12.486(2), c 11.038(2) Å, β 97.15°, groupe $P2_1/n$. La bobfergusonite ressemble beaucoup aux membres du groupe de la wyllieite, mais elle s'en distingue tant par sa structure que par sa composition. Le nom honore Robert Bury Ferguson.

(Traduit par la Rédaction)

Mots-clés: bobfergusonite, nouvelle espèce minérale, phosphate, pegmatite granitique, Manitoba, wyllieite, alluaudite.

INTRODUCTION

Large crystals of a resinous brown phosphate mineral were found (by AJA) in a granitic pegmatite at Cross Lake, Manitoba. An initial electron-microprobe and X-ray-diffraction investigation of the mineral showed it to be closely related to, but distinct from, the wyllieite-group and alluaudite-group minerals. With the retirement and 65th birthday of Professor Robert Bury Ferguson at hand, and preparations underway for this special issue of *The Canadian Mineralogist,* we chose to honor our friend, colleague and teacher by naming this mineral after him. It gives us great pleasure to announce the new species *bobfergusonite.* It is particularly fitting that this new pegmatitic phosphate from Manitoba is named after Dr. Ferguson, doyen of modern mineralogy in Manitoba, in honor of his contributions to mineralogy and crystallography, many of which have focused on granitic pegmatites (*e.g., Can. Mineral.* **11**, Part 3). The new mineral and its name have been approved for publication by the IMA Commission on New Minerals and Mineral Names. Holotype material (grams) is preserved in the collections of the Mineralogical Museum, University of Manitoba, Winnipeg (M6083), and the Royal Ontario Museum, Toronto (M42687). More abundant, ideotype material is also preserved at these institutions.

LOCATION AND OCCURRENCE

The new phosphate mineral occurs in an unnamed pegmatite at Cross Lake in central Manitoba, about 5 km north-northwest of the Cross Lake settlement.

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The pegmatite, denoted #22 by Anderson (1984), is located at the southeastern shoreline of an unnamed island in the western part of the lake (Long. 54° 41′ N, Lat. 97°49′ W).

The parent pegmatite is a member of the Northern pegmatite series of the Cross Lake pegmatite field. This field is hosted by the Cross Lake greenstone belt in the Sachigo Subprovince, at the northwestern edge of the Superior Province of the Canadian Shield. Although no age determination is available for these pegmatites, they probably are of the same late Kenoran age as other fields of rare-element pegmatites in the Superior Province. Preliminary Rb/Sr isotopic data indicate a minimum age of 2.5 Ga for the leucogranites of the Cross Lake field (G.S. Clark & R.E. Meintzer, pers. comm. 1985).

Most pegmatites of the Northern series belong to the beryl–columbite type of the rare-element class of pegmatites. However, the overall geochemical signature of this series is rather exceptional among the pegmatite populations of the Superior Province. The series is poor in rare alkali metals, particularly Li and Rb relative to Cs. In contrast, enrichment in Mn and F is noticeable in the most fractionated members of the series, such as the #22 pegmatite (Anderson 1984).

PARAGENESIS

The #22 pegmatite is emplaced in metagreywacke, which grades into metaconglomerate south of the dyke. The main part of the pegmatite is 40 m long and up to 6.7 m wide in outcrop, with prominent but asymmetric zoning. The wall zone, adjacent to the northwestern contact, consists mainly of saccharoidal albite and quartz, with scattered garnet, schorl, muscovite and K-feldspar. The same mineral assemblage dominates the outer intermediate zone, in which it is accompanied by columbite–tantalite, microlite, apatite, and beryl. Large crystals of brown K-feldspar and book muscovite form the inner intermediate zone, separated from a segmented quartz "core" by core-margin muscovite and columnar green beryl. The quartz "core" is in contact with the wallrock along the southeastern flank of the pegmatite.

Phosphate minerals most commonly occur as nodules in the intermediate zones of the pegmatites; however, large, isolated crystals of bobfergusonite with no associated phosphates are also present. The nodules consist of intimately associated primary phosphate minerals, which show little or no replacement by secondary phosphates. These primary phosphate minerals are bobfergusonite, beusite, fillowite, triplite, apatite, and an unknown Mn-phosphate. Very minor alluaudite is also present, and is probably secondary in origin.

The phosphate assemblage is unique for its diversity and extreme Mn-enrichment. Assemblages of primary phosphate minerals in granitic pegmatites are typically much less diverse, and not as intimately associated, the minerals occurring most typically as large isolated crystals. All of the primary phosphates present are the examples richest in Mn known for their species, and have very high values of Mn/(Mn + Fe^{2+}). The assemblage will be dealt with in greater detail in a later paper, when all of its members have been more completely characterized.

PHYSICAL AND OPTICAL PROPERTIES

Bobfergusonite typically occurs as anhedral, equant single crystals, or as aggregates of relatively few crystals. Crystal size ranges from less than 1 mm to 1 cm long. The mineral is variable in color, ranging from green-brown to red-brown. The red-brown variety was initially perceived to be volumetrically the most significant, so representative red-brown material was designated as the holotype. All data presented in this paper pertain to the holotype, unless otherwise stated.

All color varieties are nonfluorescent and have a yellow-brown streak. The mineral is brittle, shows perfect {010} cleavage and has a prominent {100} parting. The lustre is resinous except on the parting surface, which shows a characteristic bronzy lustre. The measured density is 3.54(1) g/cm^3, based on five repeated weighings with a Berman balance; the mean calculated density of 3.57 g/cm^3 agrees well with the measured value. The hardness is 4.

Small chips of the mineral are transparent. Bobfergusonite is biaxial positive. Indices of refraction were measured by the Becke line method with the use of a spindle stage and a Na-light source (589 nm): α 1.694(1), β 1.698(1), γ 1.715(2). The $2V$ angle, determined from extinction curves refined from spindle-stage data using the program EXCALIBR (Bloss 1981), is 46.4(2)°, which compares well with $2V$(calc) 52°. The optic orientation is $Y \| b$ and $a \wedge X = +10°$ in the β angle. Pleochroism is moderate: $X = Y$ yellow-orange, Z orange. Absorption: $Z > X \simeq Y$. Using the Gladstone–Dale constants of Mandarino (1981), the compatibility index is 0.014, indicating superior agreement between physical and optical data.

X-RAY CRYSTALLOGRAPHY

Precession photographs of bobfergusonite are very similar to those of the wyllieite-group minerals, except for the presence of large numbers of diffraction spots at ½ h and ½ l (wyllieite cell), suggesting that the bobfergusonite structure is a derivative of the wyllieite structure. The cell volume is four times that of the wyllieite structure; however, a and c can be reset to give a unit cell with only twice the volume of the wyllieite structure. This cell has dimensions $a \simeq 12.8$, b 12.5, c 11.0 Å, β 97.5°, and is related to the setting chosen for the wyllieite cell (Moore & Ito 1973) by: $a(\mathrm{B}) = 2c(\mathrm{W})$, $b(\mathrm{B}) = b(\mathrm{W})$, $c(\mathrm{B}) = a \bullet \sin \beta / [(101)^* \wedge (200)^*]$ (W), and $\beta(\mathrm{B}) = [(101)^* \wedge (200)^*]$ (W). B and W stand for bobfergusonite and wyllieite, respectively. Systematic absences are $h0l$ with $h + l = 2n + 1$ and $0k0$ with $k = 2n + 1$, uniquely giving $P2_1/n$ as the space group.

Unit-cell dimensions for bobfergusonite, obtained by single-crystal X-ray diffractometry (Mo$K\alpha$ radiation), are given in Table 1. One green-brown and two red-brown crystals were investigated. Unit-cell dimensions vary slightly with color: the red-brown variety tends to have smaller a and b cell edges than the green-brown variety, yet c and β of both varieties are similar.

X-ray powder diffractograms of bobfergusonite are very similar to those of the wyllieite-group and alluaudite-group minerals (Table 2). The wyllieite structure is a more highly ordered derivative of the alluaudite structure, and the bobfergusonite structure is a more highly ordered derivative of the wyllieite structure (Ercit *et al.* 1986). Consequently, it is of little surprise that diffraction maxima corresponding to the alluaudite-structure subcell are strong in the powder patterns of all three types of structure and dominate their diffraction records. From the data of Table 2, the supercell diffraction-maxima of wyllieite have a mean relative intensity of only 2% and, except for (100), with an intensity of 6%, are difficult to detect without modern X-ray equipment (1.5 kW X-ray tubes or better). The diffraction maxima of bobfergusonite that violate the symmetry of wyllieite are necessarily even weaker than the supercell diffraction-maxima of the wyllieite structure, and cannot be observed by powder methods. Consequently, in X-ray-diffraction investigations, bobfergusonite can only be confidently distinguished from wyllieite-group and alluaudite-group minerals by single-crystal methods.

To simplify distinction by single-crystal methods, the cell chosen by Moore & Ito (1973) for the alluaudite-group and wyllieite-group minerals was transformed to the bobfergusonite setting, which involves no change in the cell volume. On the bobfergusonite setting, the cells for the three structure types are of comparable dimensions except for a: $a(\mathrm{A}) = a(\mathrm{W}) = \frac{1}{2}a(\mathrm{B})$. However, on this common setting, the space groups of these structures are different: the alluaudite structure has $I2/a$, the wyllieite structure has $P2_1/c$, and bobfergusonite has $P2_1/n$. This setting was used in indexing the patterns of Table 2.

TABLE 1. UNIT-CELL DIMENSIONS FOR 808FERGUSONITE

	Red-brown		Green-brown
	P-1	P-8	P-2
a (Å)	12.776(2)	12.797(2)	12.843(3)
b	12.488(2)	12.478(2)	12.518(3)
c	11.035(2)	10.996(2)	11.014(2)
β (°)	97.21(1)	97.47(1)	97.37(2)
V (Å³)	1746.7(4)	1741.0(5)	1756.0(6)

Determined using a Nicolet R3m four-circle diffractometer with graphite-monochromated MoKα radiation.

The structure types can be distinguished on the basis of a single $(h0l)^*$ precession photograph, which is quite easy to obtain because all three groups of minerals have only {010} as a perfect cleavage. A schematic composite $(h0l)^*$ precession photograph is shown in Figure 1. Minerals with the wyllieite structure (upper right-hand quadrant of Fig. 1) can be distinguished from those with the alluaudite structure (upper left-hand quadrant of Fig. 1) by the presence of extra diffraction-maxima with h odd, which halve the apparent 0-level repeat period for alluaudite along X. In turn, bobfergusonite (lower half of Fig. 1) can be distinguished from wyllieite-group minerals by the presence of additional diffraction-maxima that halve the apparent 0-level repeat periods along both X and Z of wyllieite (and thus quarter and halve the apparent 0-level X and Z repeat periods of alluaudite).

CHEMISTRY

Energy-dispersion X-ray spectra were obtained with a MAC 5 electron microprobe using a Kevex Micro-X 7000 spectrometer. Spectra were collected for 200 live seconds with an operating voltage of 15 kV and a sample current of 10 nA (measured on synthetic fayalite), and were corrected for current and voltage drift. $\mathrm{NaInSi_2O_6}$ (Na), chromite (Mg,Al,Fe), apatite (P,Ca), $\mathrm{MnF_2}$ (Mn) and willemite (Zn) were used as standards.

Data were reduced with Kevex software utilizing the program MAGIC V (Colby 1980). P$K\alpha$ overlap onto Al$K\alpha,\beta$ due to incomplete charge-collection, Zn$L\alpha,\beta$ overlap onto Na$K\alpha,\beta$, and Mn$K\beta$ overlap onto Fe$K\alpha$ were dealt with by stripping techniques using library spectra acquired at the same time as the sample spectra.

The $\mathrm{Fe^{2+}/Fe^{3+}}$ ratio was determined by ^{57}Fe-Mössbauer spectroscopy. Spectra were collected with a 512-register multichannel analyzer on samples containing an Fe-concentration of 5 mg/cm^2, and were folded to give 245 data points over an approximate range of –4 to +4 mm/s (relative to α-Fe foil). Data were collected on red-brown holotype material and on a representative sample of the green-brown variety. Resulting values of the $\mathrm{Fe^{2+}/Fe^{3+}}$ ratio were determined from areas of the spectral components (Ercit *et al.*, in prep.); 0.05 was found for the red-brown variety and 0.54 for the green-brown variety.

Examination of a 23-mg sample of the holotype by thermogravimetry indicated the presence of minor amounts of H_2O and CO_2. H_2O was evolved between 70 and 400°C, peaking at 90 and 300°C. CO_2 was evolved between 400 and 600°C, peaking at 540°C. The data for H_2O evolution are similar to those for the mineral O'Danielite (Keller *et al.* 1981a), a relative of alluaudite-group minerals that contains O–H bonds (Keller *et al.* 1981b). Consequently, the H_2O evolved from bobfergusonite (0.28 wt.%) is interpreted to represent OH in the structure. The very minor CO_2 (0.17 wt.%) is most probably due to contamination.

Results of analyses of five spots across a 3-mm cleavage fragment of the red-brown holotype are given in Table 3. The data show that the mineral is homogeneous over the scale of a crystal. Only Zn appears to violate this observation; it is present at only one of the five spots. The detection limit for Zn is approximately 0.25 wt.% ZnO; it is possible that Zn may also vary only slightly, but being near its detection limit, its variation may seem to be more extreme than is actually the case. Results of two analyses taken from a 1-mm crystal of a typical sample of the green-brown variety are also given in Table 3. They show that the mineral does vary in chemistry from grain to grain, despite intragranular homogeneity. The green-brown variety has a higher Fe^{2+}/Fe^{3+} ratio, higher total Fe and slightly lower Al than the red-brown variety.

Formula contents for averaged compositions (Table 4) were calculated on a basis of 24 (O + OH). Consideration of the density and unit-cell volume gives $Z = 4$ for this basis. Cation sums for both varieties are appreciably lower than 16, the maximum number of cations possible in the wyllieite and alluaudite structures on a basis of 24 (O + OH). The sums closely approach 15, suggesting that bobfergusonite ideally has one vacancy per formula unit.

Strictly empirical formulae are difficult to calculate for alluaudite-group and wyllieite-group minerals and bobfergusonite owing to disorder of some of the cations in these minerals over several sites, *e.g.*, Mn disorder over several of the *M* and *X* sites. Consequently, semiempirical formulae must be calculated.

Results of the crystal-structure analysis (Ercit *et al.* 1986) give the structural formula of bobfergusonite as:

$$[X5_4X4_4][X3_2X2_2]X1_4\,[M1_4M2_4][M3_4M4_4]M5_4M6_4(PO_4)_{24}$$

where *X*2–*X*5 are occupied by Na, □, *X*1 by Mn, (Ca), *M*1 and *M*2 by Mn, (□), *M*3 and *M*4 by Mn, (Fe^{3+},Al), *M*5 by Fe^{3+}, Al, (Mg, Zn, Fe^{2+}), and *M*6 by Al, (Fe^{3+}).

TABLE 2. POWDER-DIFFRACTION DATA FOR BOBFERGUSONITE AND RELATED MINERALS

Bobfergusonite (P-1)[1]				Ferrowyllieite[1]			Hagendorfite[2]		
hkl	d (calc)	d (obs)	I	hkl	d (obs)	I	hkl	d (obs)	I
011	8.23	8.24	6	011	8.09	13	011	8.16	2
200	6.34	6.33	18	100	6.26	6			
020	6.24	6.26	9	020	6.14	20	020	6.26	21
002	5.48	5.47	6	002	5.39	10	002	5.40	6
$\bar{2}11$	5.27	5.26	4	$\bar{1}11$	5.20	2			
012	5.01	5.01	1						
211	4.81	4.81	2	111	4.74	1			
220	4.447	4.445	3	120	4.388	2			
$\bar{2}21$	4.252	4.254	2				$\bar{1}21$	4.286	2
$\bar{2}12$	4.171	4.171	4	$\bar{1}12$	4.120	4	$\bar{1}12$	4.188	8
022	4.117	4.120	5	022	4.052	6	022	4.094	3
							121	4.003	1
				$\bar{1}22$	3.565	1			
013	3.504	3.506	16	013	3.452	30	013	3.462	22
230	3.479						130		
231	3.385	3.383	2	131	3.337	4			
				122	3.263	1			
				113	3.193	2			
$\bar{4}11$	3.054	3.054	100	$\bar{2}11$	3.025	22	$\bar{2}11$	3.093	44
				$\bar{1}32$	2.993	6	$\bar{1}32$	3.042	9
$\bar{2}23$	2.951	2.952	4	$\bar{1}23$	2.912	3			
$\bar{4}02$	2.904	2.902	37	$\bar{2}02$	2.875	9	$\bar{2}02$	2.937	16
411	2.868	2.869	66	211	2.833	27	211	2.881	41
420	2.825	2.824	36	220	2.791	19	220	2.849	15
$\bar{2}41$	2.750			$\bar{1}41$	2.698	57	$\bar{1}41$	2.762	15
004	2.738	2.739	36	004			004	2.707	100
042	2.711	2.712	49	042	2.711	100	042		
$\bar{4}22$	2.633	2.633	20	$\bar{2}22$	2.605	9	$\bar{2}22$	2.660	[illegible]
402	2.606	2.607	17	202	2.572	7	202	2.601	1[illegible]
$\bar{2}14$	2.578	2.579	2				$\bar{1}14$	2.564	3
$\bar{2}42$	2.551	2.551	2	$\bar{1}42$	2.515	3			
$\bar{4}32$	2.512			$\bar{2}31$	2.479	27	$\bar{2}31$	2.534	43
024	2.507	2.508	53	$\bar{2}13$			$\bar{2}13$		
$\bar{4}13$	2.504						024	2.480	7
422	2.405	2.405	10	222	2.371	7	222	2.403	6
250	2.323	2.324	2	150	2.289	3	150	2.333	5
$\bar{2}43$	2.283	2.283	2						
$\bar{2}34$	2.227	2.224	3	$\bar{1}34$	2.196	4	$\bar{1}34$	2.220	2
				213					
$\bar{4}33$	2.178	2.178	10	$\bar{2}33$	2.152	8	$\bar{2}33$	2.192	4
015	2.157	2.158	7	015	2.126	11	015	2.128	11
610	2.083	2.082	67	310	2.061	15	310	2.103	34
060	2.081			060	2.053	5	060	2.088	5
053	2.061	2.061	6	053	2.029	10	053	2.056	9
442	2.000	2.001	5				242	2.002	2
433	1.985	1.985	8	233	1.956	7	233	1.976	9
404	1.954	1.954	4				062		
062	1.947	1.945	4	062	1.911	8	204	1.946	8
035	1.938	1.936	4	035			035	1.918	6
630	1.884	1.883	4				330	1.899	4
							125	1.876	2
424	1.866	1.865	4	224	1.839	6	224	1.850	2
$\bar{2}54$	1.813	1.813	4	$\bar{1}54$	1.787	4	$\bar{1}54$	1.811	6
$\bar{2}16$	1.796	1.796	4	$\bar{1}16$	1.772	6	$\bar{1}16$	1.780	7
$\bar{4}53$	1.786	1.786	2	$\bar{2}53$					
$\bar{6}41$	1.756	1.755	4	$\bar{3}41$	1.736	3	$\bar{3}41$		
$\bar{4}35$	1.741	1.741	13	$\bar{2}35$	1.718	11	$\bar{2}60$	1.744	15
460	1.739			260			235		
270	1.717	1.717	3	170	1.691	3	170	1.724	5
$\bar{4}62$	1.691	1.690	2	$\bar{2}62$	1.665	2			
$\bar{4}15$	1.690			$\bar{2}15$			$\bar{2}15$		
245	1.681	1.678	4	145	1.653	3	323	1.670	4
623	1.673			323			145		
444	1.657	1.657	7	244	1.632	6	$\bar{3}34$	1.648	13
				$\bar{3}34$	1.623	4	244		
				055					
$\bar{4}26$	1.617	1.617	6	$\bar{2}26$	1.597	6	350	1.625	4
650	1.613			350			$\bar{2}26$	1.615	3
$\bar{6}52$	1.589	1.588	4	$\bar{3}52$	1.571	3	$\bar{3}52$		
$\bar{8}11$	1.583	1.583	6	$\bar{4}11$	1.561	9	$\bar{4}11$	1.598	15
046	1.576	1.575	43	$\bar{4}02$			$\bar{4}02$		
$\bar{8}02$	1.575			046	1.553	15	046	1.561	10

SG: $P2_1/n$	SG: $P2_1/c$	SG: $I2/a$
a: 12.773(2) (Å)	a: 6.323(1)	a: 6.464(1)
b: 12.486(2)	b: 12.293(2)	b: 12.527(1)
c: 11.038(2)	c: 10.880(2)	c: 10.907(1)
β: 97.15(1) (°)	β: 97.35(1)	β: 97.93(1)

1. Victory Mine, South Dakota, USA.
2. Hagendorf-south Mine, W. Germany.

Philips PW1710 automated powder diffractometer, automatic divergence slit, graphite-monochromated CuKα radiation. Internal standard: NBS silicon, batch 640a.

Positions over which there is complete disorder are enclosed in brackets. *M*- and *X*-site constituents of lesser abundance are enclosed in parentheses. Grouping the contents of the *M* sites *versus* the *X* sites gives the semiempirical formula ($Z = 4$):

$$(Na_{2.04}Mn_{0.53}Ca_{0.20}\square_{1.20})_{\Sigma 4}(Mn_{3.68}Al_{1.39}Fe^{3+}_{0.81}Mg_{0.07}Fe^{2+}_{0.04}Zn_{0.01})_{\Sigma 6}P_{5.99}(O_{23.69}OH_{0.31})_{\Sigma 24}$$

which, disregarding minor *M*-site vacancies, is calculated by assigning all Al, Fe, Mg, Zn to the *M* sites, together with enough Mn to sum to 6 cations. The remaining Mn plus all Na and Ca are assigned to the *X* sites.

The presence of a large number of vacancies at the *X* sites is a response to excess positive charge at the *X* and *M* sites owing to the presence of Mn at *X*1 and minor Al^{3+} at *M*3 and *M*4.

Ideal bobfergusonite has only Mn at *M*1–*M*4 and *X*1, Fe^{3+} at *M*5, Al at *M*6, only Na at *X*2–*X*3, and 1:1 Na:□ at *X*4–*X*5 (Ercit *et al.* 1986). The ideal formula is thus: $Na_2Mn_5Fe^{3+}Al(PO_4)_6$ ($Z = 4$).

DISCUSSION

Bobfergusonite is closely related to the alluaudite-group and wyllieite-group minerals. The three structure-types differ principally in terms of cation ordering within and between chains of *M*-cation octahedra (Ercit *et al.* 1986). The alluaudite structure shows the least amount of cation ordering, ranging from having complete *M*-cation disorder (*e.g.*, end-member varulite) to two-site *M*-cation chain order (*e.g.*, end-member alluaudite). The wyllieite structure shows greater intrachain cation order; cation ordering takes place over two sets of *M* sites (*e.g.*, end-member ferrowyllieite) to a maximum of three *M* sites (*e.g.*, end-member wyllieite). The bobfergusonite structure shows ordering of wyllieite-like intrachain cations over four sets of *M* sites, with a potential maximum of up to six sites.

Moore & Ito (1979) have subdivided the alluaudite and wyllieite groups on the basis of cation partitioning between certain *M* sites. Table 5 summarizes the method of classification and lists presently known species. Extending the classification criteria to bobfergusonite, the population of *M*1 + *M*2 corresponds to the *A* criterion, and the population of *M*3 + *M*4 corresponds to the *B* criterion of Table 5. Bobfergusonite has Mn dominant for both criteria, thus its alluaudite-group analogue is varulite, but it has no known wyllieite-group analogue. Although bobfergusonite would seem to be very similar to varulite according to the criteria of Table 5, it has major amounts of Al, unlike varulite.

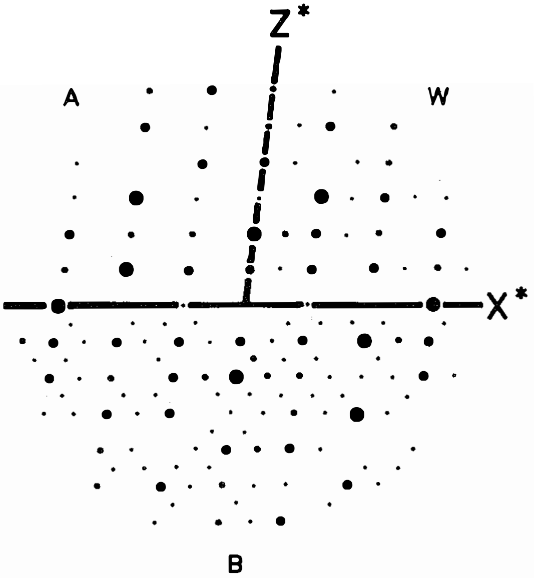

FIG. 1. A schematic composite (*h*0*l*)* precession photograph showing the differences in the diffraction patterns of the alluaudite structure (*A*, upper left-hand quadrant), the wyllieite structure (*W*, upper right-hand quadrant) and the bobfergusonite structure (*B*, lower half). Spot size mimics diffraction intensity; the smallest spots cover the 1–25% intensity range, intermediate spots cover the 26–50% and 51–75% ranges, and the largest spots cover the 76–100% range.

TABLE 3. CHEMICAL COMPOSITION OF BOBFERGUSONITE

		Red-Brown (P-1)					Green-Brown (P-2)	
		1	2	3	4	5	1	2
Na_2O	wt.%	6.7	7.0	7.0	6.6	6.8	6.5	6.1
MgO		0.3	0.3	0.4	0.3	0.4	0.4	0.5
CaO		1.2	1.1	1.3	1.3	1.3	0.6	0.6
MnO		31.5	32.0	31.9	31.3	31.8	32.7	31.8
FeO		0.3	0.3	0.3	0.3	0.3	3.4	3.7
ZnO		0.5	0.0	0.0	0.0	0.0	0.2	0.4
Al_2O_3		7.5	7.5	7.5	7.4	7.6	5.2	4.6
Fe_2O_3		6.7	6.8	7.1	6.6	7.0	7.1	7.6
P_2O_5		45.3	45.7	45.4	44.7	45.3	43.8	43.7
H_2O		0.3	0.3	0.3	0.3	0.3	0.3	0.3
		100.3	101.0	101.0	98.8	100.8	100.2	99.3

For sample P-1, 1 to 3 pertain to the core, and 4,5 to the rim. For P-2, 1 pertains to the core, and 2 to the rim.

All elements with Z>10 were determined by electron microprobe. H_2O is based on a single TG analysis for sample P-1. Fe^{2+}/Fe^{3+} is obtained by Mössbauer spectroscopy for one sample each of P-1 and P-2.

TABLE 4. AVERAGED FORMULA CONTENTS OF BOBFERGUSONITE

Sample	Na	Mg	Ca	Mn	Fe^{2+}	Zn	Al	Fe^{3+}	P	OH	O
P-1	2.07	0.07	0.20	4.21	0.04	0.01	1.39	0.81	5.99	0.31	23.69
P-2	1.98	0.10	0.10	4.41	0.49	0.04	0.93	0.89	6.00	0.32	23.68

Calculated on a basis of 24(O+OH) from averages of the analyses of Table 3. Cation sums: P-1 14.79, P-2 14.94.

TABLE 5. CLASSIFICATION OF ALLUAUDITE- AND WYLLIEITE-GROUP MINERALS*

Dominant Cation A	Dominant Cation B	Alluaudite Group	Wyllieite Group
Mn^{2+}	Fe^{2+}	Hagendorfite	Wyllieite
Fe^{2+}	Fe^{2+}	---	Ferrowyllieite
Mn^{2+}	Mg^{2+}	Maghagendorfite	Qingheiite
Fe^{2+}	Mg^{2+}	---	---
Mn^{2+}	Mn^{2+}	Varulite	---
Fe^{2+}	Mn^{2+}	(us.)	(us.)
Mn^{2+}	Fe^{3+}	Alluaudite	Rosemaryite
Fe^{2+}	Fe^{3+}	Ferroalluaudite	---

A: M1 site, B: M2 site for alluaudite-group minerals.
Ā: M1 site, B̄: M2a site for wyllieite-group minerals.

The generic name is given on the basis of the identity of B. The identity of A determines the prefix: if Mn is dominant, no prefix; if $Fe^{2+}$is dominant, "ferro" is used. Maghagendorfite is an exception.

---: not yet known, us.: predicted to be unstable, * modified after Moore & Ito (1979).

It would seem at the present time that bobfergusonite can be distinguished from all known wyllieite-group and alluaudite-group minerals on the basis of chemistry alone. Although these differences in chemistry presently are known, it is possible that a wyllieite-group analogue of bobfergusonite may be found in the future. Because of the similar Al-contents of bobfergusonite and the wyllieite-group minerals (*cf.* Moore & Ito 1979), distinction on the basis of chemistry alone may eventually not be possible; however, the use of both chemical and structural (*i.e.*, single-crystal XRD) data will always give an unambiguous identification.

ACKNOWLEDGEMENTS

We thank R.A. Ramik of the Royal Ontario Museum for the TG analysis, and C.A. McCammon, formerly of the Dept. of Physics, University of Manitoba for the collection of Mössbauer spectra. We extend thanks to the following members of the Department of Earth Sciences, University of Manitoba, for their contributions: R. Chapman obtained some of the first ED X-ray spectra of the mineral, and R. Eby obtained unit-cell parameters for the green-brown variety by single-crystal diffractometry. Financial support for this work was provided by Natural Sciences and Engineering Research Council of Canada operating grants to PC and FCH, and by the Canada–Manitoba Interim Agreement on Mineral Development, 1982–1984.

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Received October 23, 1985, revised manuscript accepted September 17, 1986.