MINERALOGICAL MAGAZINE

VOLUME 42 NUMBER 323 SEPTEMBER 1978

I. Whiteite, a new species, and a proposed nomenclature for the jahnsite-whiteite complex series. II. New data on xanthoxenite. III. Salmonsite discredited.

PAUL BRIAN MOORE AND JUN ITO*

Department of the Geophysical Sciences, The University of Chicago, Chicago, Illinois 60637, U.S.A.

SUMMARY. Whiteite, $Ca(Fe,Mn)^{2+}Mg_2Al_2(OH)_2$ (H₂O)₈[PO₄]₄, *a* 14:90(4) Å, *b* 6:98(2) Å, *c* 10:13(2) Å, β 113° 07(10)', Z = 2, space group P2/a, α 1:580(5), β 1:585(5), γ 1:590(5), 2V 40-50°, specific gravity 2:58, is a new species from the Ilha de Taquaral, Minas Gerais, Brazil. It is the Al³⁺-analogue of jahnsite. The mineral occurs as up to 5 mm tan crystals flattened on {001}. Twinning by reflection on {001} leads to pseudoorthorhombic development. Rather pure material also occurs from Blow River, Yukon Territory, Canada.

For the general formula $XM(1)M(2)_2M(3)_2(OH)_2$ (H₂O)₆[PO₄]₄, it is proposed that for M(3), Al³⁺ > Fe³⁺, the established members of the series are whiteite—(CaFe²⁺Mg) and whiteite—(Mn²⁺Fe²⁺Mg); and for Fe³⁺ > Al³⁺, jahnsite—(CaMn²⁺Hg), jahnsite—(CaMn²⁺Fe²⁺), and possibly jahnsite—(Mn²⁺Mn²⁺Mn²⁺).

Xanthoxenite of Laubmann and Steinmetz (1920) is probably stewartite (in part) on the basis of morphological, optical, physical, and paragenetic evidence. The xanthoxenite of Frondel (1949) is proposed as the species type. It is triclinic, $P\bar{1}$ or PI, $a \ 6.70(4)$ Å, b8.85(4) Å, $c \ 6.54(3)$ Å, $\alpha \ 92.1(2)^{\circ}$, $\beta \ 110.2(2)^{\circ}$, $\gamma \ 93.2(2)^{\circ}$, Z = Ifor composition $Ca_4 Fe_2^{-1} + (OH)_2(H_2O)_3[PO_4]_4$.

Salmonsite, c. $Mn_3^{-2} Fe_2^{-1}(PO_4)_8.14H_2O$, from Pala, California, is shown to be an intimate mixture of hureaulite and jahnsite on the basis of calculated and observed powder patterns and on reinterpretation of the original chemical analysis published by Schaller (1912). It is a breakdown product resulting from oxidation of Fe^{2+} in the original hureaulite ('palaite') along with further aquation followed by fine-grained recrystallization. The reaction proposed is:

$$\begin{array}{l} (Mn_{0\cdot85}Fe_{0\cdot15})_{5}^{2+}(H_{2}O)_{4}[PO_{3}OH]_{2}[PO_{4}]_{2} + \\ I \cdot I2H_{2}O + 0.4I \ O_{2} \rightarrow \\ & \text{`palaite'} (= \text{hureaulite}) \\ 0.55Mn_{5}(H_{2}O)_{4}[PO_{3}OH]_{2}[PO_{4}]_{2} + \\ & \text{hureaulite} \\ 0.75Mn_{2}^{2+}Fe^{3+}(OH)(H_{2}O)_{4}[PO_{4}]_{2} + 0.30PO_{4}^{3-} \\ & \text{jahnsite.} \end{array}$$

PROVIDED herein are data on a new species, whiteite, which is the Al member of the jahnsite, $CaMn^{2} + Mg_2Fe_2^{3} + (OH)_2(H_2O)_8[PO_4]_4$, structure type. During this study several difficult problems arose concerning nomenclature and definition of species, and it became evident that this study could not be split into separate contributions. Owing to variable oxidation states and gross similarities in physical properties, the basic aluminum and ferric phosphates discussed in this study are among the most perplexing in descriptive mineralogy and a detailed survey of the earlier literature on some of these compounds was also necessary.

Whiteite Ca(Fe,Mn)²⁺Mg₂Al₂(OH)₂(H₂O)₈[PO₄]₄ (formula of the type)

* Died 6 June 1978.

Descriptive mineralogy. Numerous specimens from Ilha de Taquaral in the State of Minas Gerais, Brazil, have appeared on the dealer's market that show abundant large childrenite-eosphorite crystals and smaller amounts of wardite and a green botryoidal phase related to roscherite attractively grouped upon large rose quartz crystals and along joints and fractures in quartz and albite. Occasional specimens provide a pale tan to brown mineral occurring as bunched aggregates of small (I-5 mm) tabular crystals to large (up to 2 cm) thick tabular canoe-shaped individuals.

The paragenesis is interpreted as a moderatetemperature hydrothermal vein association where subordinate alkalis, alkaline earth, and transition metals and major aluminium and phosphate afforded a series of basic aluminium phosphates. It is likely that cations such as Fe^{2+} , Mn^{2+} , and Be^{2+} were derived from pre-existing primary phases, perhaps beryl and triphylite–lithiophilite, which were earlier attacked by the aqueous-rich fluid separate formed during core consolidation and their cations selectively leached and subsequently transported elsewhere to open fissures.

The new species, whiteite, is pale tan (the type) to chocolate brown (the Ca-poor variant) and nearly colourless in small fragments. The hardness is 3 to 4 and the cleavage is {001} good to perfect. The specific gravity for the pale tan type is 2.58(1) and for the Ca-poor variant 2.67(2), both determinations made on the Berman torsion balance with toluene as the displaced fluid at 21 °C.

Crystal morphology. Both whiteite and its Capoor variant occur as warped crystals showing the forms $c\{001\}$ and $n\{\bar{1}11\}$. These crystals are invariably twinned by reflection on $\{001\}$, imparting a pseudo-orthorhombic appearance to the composite. For the type, $c\{001\}$ is very large and affords tabular crystals with a rhombus-shaped outline whose acute angle in the plan view is 50° 04' (fig. 1). These crystals range from 1 to 5 mm in greatest dimension.

The Ca-poor variant consists of crystals up to 1.5 cm in length where the areas of $c\{001\}$ and $n\{\bar{1}11\}$ are nearly balanced, affording a canoe-shaped outline to the crystals. This appearance is made more pronounced by the curved aspect of the $n\{\bar{1}11\}$ facets resulting in an almond-shaped cross-section. The structural basis for twinning in the whiteites is advanced in the next section.

X-ray crystallography. Single crystals of type whiteite and its Ca-poor variant were studied by rotation, Weissenberg, and precession photography. In addition, crystals were ground with glass and powder diffractometer traces were obtained (I° min⁻¹ in 2 θ ; Cu-K_a radiation with graphite monochromator). Owing to relatively few strong

reflections and frequent near-coincidence of the planes, considerable difficulty was encountered in unambiguously indexing these data. To overcome the uncertainties of Miller index assignment, the strong single crystal intensities were used as a guide. This was achieved by utilizing the atomic coordinate parameters in Moore and Araki (1974a) from which calculated powder patterns could be directly obtained. This calculation was also done for the whiteite member by assuming perfect isomorphic replacement. Built into the least-squares programme is an option to correct for absorption effects; the observed data reported in Table I, however, constitute the initial input for these have most meaning in routine powder diffractometry as a determinative tool. The indexed powder data (Table I) were then used to obtain the single-crystal results (Table II) by least-squares refinement. These were in turn used to calculate the d-spacings. Of the possible single-crystal intensities, only about 10% are sufficiently strong to appear on diffractometer traces and, consequently, the powder patterns deceptively suggest a simple compound. Due to considerable overlap of intensities arising from non-equivalent planes, the least-squares convergences are not as precise as expected for a crystal structure of moderate complexity.

The single-crystal photographs clearly revealed the twinned character of both white te samples, and the photographs could be interpreted on the basis

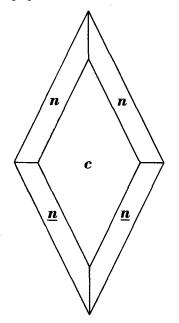


FIG. 1. Plan of white twinned by reflection on $\{001\}$ showing the forms $c\{001\}$ and $n\{\overline{1}11\}$. Taquaral pegmatite.

of the jahnsite crystal structure reported by Moore and Araki (1974a). Define c' = 2c + a/2, and cos $\beta' = [a/2)^2 - (c')^2 - (2c)^2]/ac'$. The pseudo-orthorhombic criteria are then a, b, c', and β' , and Table II shows that β' is in the range $90 \pm 2^\circ$. Presumably, the closer β' is to orthogonality, the greater the likelihood of twinning.

Chemical composition. Both type whiteite and its calcium-poor variant were examined by electronmicroprobe analysis, the refined results of which are presented in Table III as analyses 1a and 5. As in the jahnsite study of Moore (1974a), here repeated as analysis 6a, the oxide percentages are all slightly low and formula compositions are based on P = 4, that is, half the unit-cell contents. Since the structure type and atomic positions are known (Moore and Araki, 1974a), the problem reduces to a site distribution compatible with the general formula, $XM(1)M(2)_2M(3)_2^{3+}(OH)_2(H_2O)_8[PO_4]_4,$ where X accommodates the largest cations such as Ca^{2+} , Mn^{2+} , minor Na^+ , etc.; M(I) accommodates Mn^{2+} and Fe^{2+} ; M(2) accommodates Mg^{2+} , Mn^{2+} , Fe^{2+} , and even Mn^{3+} and Fe^{3+} (for highly oxidized material); and M(3) accepts Al³⁺ and Fe^{3+} . In this formula the M cations are in distorted octahedral coordination. In whiteites as in the jahnsites all water molecules and hydroxyl groups are bound to cations in the structure and are assumed to be quantitatively present. We propose the following distributions:

	Whiteite (type)	Whiteite (Ca-poor)
X	$Ca_{0.9}^{2+}Mn_{0.1}^{2+}$	$Mn_{0.8}^{2+}Ca_{0.2}^{2+}$
<i>M</i> (1)	$Fe_{0.7}^{2+}Mn_{0.3}^{2+}$	$Fe_{0.9}^{2+}Mn_{0.1}^{2+}$
M(2)	$Mg_{1\cdot 0}^{2+}$	$Mg_{1:0}^{2+}$
M(3)	$Al_{1\cdot 0}^{3+}$	$Al_{1\cdot 0}^{3+}$
ρ (calc.,	2.21	2.62
g cm ⁻	3)	

It is tempting to suggest that the Ca-poor variant formed earlier and recovered the Mn^{2+} cations in solution. At a later stage, when nearly all Mn^{2+} was removed from the fluid, the Ca²⁺-rich phase crystallized. This is consistent with the observation that the Ca-poor variant occurs as large crystals and its growth probably spanned a longer period of time.

As this paper was completed and ready for submission, Mr. Gunar Penikis of Toronto submitted three samples of tentatively identified whiteite from the Blow River, Yukon Territory, Canada, a locality that has become a source of unusual phosphate species and recently described by Mandarino and Sturman (1976). The specimens were sections of coarse crystals, tan to grey in colour and much resembling albite in appearance, and of sufficient quantity to warrant complete wetchemical analyses. The results, given in Table III as

analyses 2, 3, and 4, confirm the general formula for the whiteite-jahnsite series and are in excellent agreement with theoretical cation contents in the formula unit. These three samples belong to white $-(CaFe^{2+}Mg)$. A powder pattern from the sample used for analysis 2 is given in Table I and is in general agreement with type whiteite. Mr. Penikis informs us that the sample representing analysis 2 came from an 'A-vein', analysis 3 from a 'B-vein and found in 1974', and analysis 4 from a 'special type vein found two miles down from the main campsite in 1976 and associated with lustrous siderite and lazulite'. Since our specimens are only sections of crystals it is not possible to reconstruct the detailed paragenetic setting at these occurrences.

Optical data for the two whiteites and the jahnsites that have been studied in detail are summarized in Table IV.

Namé. It is fitting to christen the new species, after Mr. John S. White, Jr., Editor of Mineralogical Record, and Associate Curator of Minerals and Gems, the U.S. National Museum of Natural History. His liaison between amateur and professional communities has provided many examples of fine specimens for research that otherwise would have passed unnoticed and he has played a major role in the renaissance of mineralogy as an amateur as well as professional pursuit. The type specimens are preserved in the U.S. National Museum of Natural History collections.

The jahnsite-whiteite series: a proposed nomenclature

We propose that M(3) distinguishes the jahnsites from the whiteites where $Fe^{3+} > Al^{3+}$ for the former and $Al^{3+} > Fe^{3+}$ for the latter. There is no evidence as yet that solid solution between the two is extensive—no such compositions have been found—but there is no structural reason to suspect why such solution could not exist.

Since the description of jahnsite by Moore (1974*a*), the species and its variants have been found at many pegmatite localities. It occurs as orange splinters intergrown with rockbridgeite, as brown warty aggregates, as yellow to greenish prismatic crystals either single or twinned and as granular orange masses. Recurrent crystal forms are $c{001}$, $a{100}$, $j{201}$, and $n{11}$. Unlike whiteite, jahnsite crystals are nearly always prismatic and striated parallel to [010]; thin tabular development has not been observed. It can be visually confounded with laueite, pseudolaueite, stewartite, childrenite, and the xanthoxenite of Frondel (1949). We have found a zero-level *b*-rotation axis Weissenberg photograph the most

	,	1																																							
	$d_{\rm calc}$	9.208	5005	166 0	5-697	5-002	4-876	4:604	4:063	3-907		3-559	3.490	3:453		3:259		3.176	2-936	2.882	2-825	2.589			2-354		2-337	2-289				1.972		1:946		1·876					
	$d_{ m obs}$	9.150	6.807	160.0	6-639	4.961	4-844	4.602	4.059	3-887		3.550	5.403	3:451		3:247		3.179	2.925	2.887	2.808	2.581			2:339		2:334	2.296				070-I		I-935		1·874					
٢	I/I_0	100	ç	2	v	25	5 S	40	IO	01		10	<u>0</u> 5	30		S		5	15	15	55	15			IO		01	S				0		01		20					
	$d_{ m obs}$	9.2 ₇	7-08	6.17	6.0 5:66	5	4.91	4.63	4.05	3-90	3.723	3-522		3.416	1	3.268		3.165	2:950		2.825	2.575	2:417		2-341			2-295	2.002			1.958		1.945		1·870	1.787	$LLL \cdot I$	1·746	1.712	699·I
9	I/I_0	IO	I	ç	1 4	-	9	4	ŝ	÷	I	S		ŝ		m		2	ŝ		8b	4	7		ŝ			7	e.			.		4		4	7	·I	6	7	I
	hkl	*100	010	007	111	210	III	002*	Ī12	310	<u>4</u> 01	<u>3</u> 12	400	402	02 I	311	220	Ž2I	401	<u>4</u> 03	022	4 21	402	Ĩ23	<u>4</u> 04	61 I	612	Ī14	422	4o3	424	$\overline{614}$	024	<u>4</u> 05	232	802	040	711	423	<u>8</u> 04	425 042
	$d_{\rm calc}$	9.322	7-140	10/	0.303 5.686	2003	4.910	4.661	4.076	3.911	3-733	3.541	3.500	3.426	3.334	3.284	3.181	3.166	2-962	2.867	2:834	2.580	2.428	2.417	2.349	2:341	2.322	2:308	2.008	2:007	1-963	096.1	1.95 I	1.948	1-946	1·866	1.785	1.776	1.750	1-713	1-710 1-667
5	I/I_0	IOO			ر ۱۱ م	L	Ĺĭ	II	5	×	I	6	TT	11	4	5	7	6 0)	81	12	47	16	7	I	ŝ	7	ŝ	I	9	7	5	7	6	ę	7	6	9	I	7	1	61 H
	$d_{\rm calc}$	9.317			6.220	5-650	10- 0	4-890	4-793	4.658	4:095		¢	3.822	3.723	3.589	3.490		3.426		3.188	3.106				2-948		2.871			2.793			2.599		2:546					
	$d_{\rm obs}$	9.30 4			6-230	5-502		4.924	4-849	4.660	4.043			3.866	3.718	3.515	3:487		3:421		3.257	3-107				2-946		2.863			2-789			2-590		2:542					
4	I/I ₀	100			۲	, K	ç	15	20	30	01			10	5	10	15		0		Į	10				20		15			65			ŝ		20					
	d_{calc}	9.312		6.99 -	0.003 6.211	5-654		4-894	4-787	4-656	4-093		4	3.831	3-746	3.599	3.510				3-191	3.104				2.960		2.879			2.787	2-702	2-614	2-597		2-549				2:424	2.357
	$d_{\rm obs}$	818.6		0009	6.214	5-598		4.922	4-824	4.644	4:036		(3-875	3.746	3.518	3:454				3.245	3.094				2:948		2-879			2-776	2-678	2-610	2.599		2.544				2:408	2.380
3	·I/I ₀	IOD		·	n v	, 6	5	20	50	40	20			20	Ş	35	30				35	×				45		. 20			8	5	0	12		25				8	8
	$d_{ m obs}$	9.270	6-899	6.800	6.18a	5.563	5	4.901	4-822	4.637	4.022		ŝ	3.853	3.697	3.498	3.476		3-402		3-246	3-094			3.026	2-941		2-849			2.781	2.643	2.615	2.582		2.535				2:412	2-381
7	I/I_0	100	S	ų	n v	, 5	2	30	65	65	20			25	Ś	35	6		25		ő	25			IO	0L		40			80	S	S	01		8				S	Ś
	hkl	*100	201		007	ĪIJ	211	210	III	002*	Ī12	<u>3</u> 11	212	310	4o1	<u>3</u> 12	<u>4</u> 02	112	400	021	311	*E00	410	121	212	<u>4</u> 03	3 13	401	<u> </u>	221	022	<u>5</u> 12	122	113	510	4 21	203	602	<u>2</u> 23	<u>4</u> 04	222 402
	d_{calc}	9.358	6-943 6-010	0.940	60.0 6-178	5.621	4-901	4.872	4.790	4-679	4-084	4.009	3.954	3-815	3.712	3.567	3:472	3:454	3.430	3:245	3.194	3.119	3.073	3-068	2.992	2-933	2-914	2-883	2.810	2:794	2.782	2-675	2.613	2-609	2.551	2.531	2.502	2.459	2.413	2:409	2:395 2:368
г	I/Io	100	Ś	4 6	v <i>v</i>	01	, m	13	30	8	6	2	m	13	ŝ	16	12	7	10	I	11	÷	ч	I	ę	16	8	20	ŝ	m	63	7	1	7	4	61	7	7	7	÷	~ ~

TABLE I. White ites and jahnsites. X-ray powder data \dagger

312

P. B. MOORE AND J. ITO

c1.	1.573																										
-	4																										
406 ∄⊺5	820																										
1-646 1-646	1-574																										
н н	. 9																										
	. 8			_						5																	
	2.328		2:313	2.064						2-006			1-987	1-951	1-937		1·862			1.735		I-634					
	2.320		2.307	2-077						2.001			1-982	I-949	1-936		1·858			1-740		1-630		1.555			1-490
	S		5	Ś						S			S	01	20		IO			5		S		15			5
2.340	2-340	2.339	2.324	2-062				2.022		2.002			689·1	1.952	I-935		1.873			1.736	1.703						
2-361	2.334	2.329	2.298	2:066				2-014		2.007			1-993	1-951	1-927		1.873			1-727	1.702		1.563	1.546		1-509	1·489
5	12	15	~	Ś				80		œ			×	15	30		25			10	80		01	15		10	01
2.339	2-318		2-296	2.073	2.039							866-1	1.982	1-943	1-929		I-854	1.792	1.733			1-635	1-556	1.552	1.528	1.516	I • 485
ŝ	10		IO	IO	5							01	01	50	15		15	S	01			S	15	45	5	5	20
213 Ī14	612	<u>6</u> 03	<u>6</u> 11	114	224	223	$\overline{3}32$	622	621	132	<u>4</u> o5	$\overline{6}$ 14	<u>4</u> 24	422	024	232	802	133	040	4 25	423	042					
2:352 2:325	2.317	2.314	2:307	2-073	2.042	2-027	2-018	2.004	866-1	266-1	266 I	1-993	LT2-1	1:954	8£6.1	1·894	1·856	1.785	1.730	1.728	1.708	1.623					
п с	. v	ŝ	ŝ	6	2	ŝ	7	6	7	7	4	e	9	9	12	e	14	7	8	2	6	6					

* Reflections enhanced by {ool}; cleavage.
 † Samples 2, 3, 4, and 7 ground with glass. Cu-K_a radiation, graphite monochromator. Scan speed 1° min⁻¹. Sample 6 from Moore (1974). Samples 3 and 4 were corrected for absorption, samples 2, 6, and 7 were not.

1. Calculated powder pattern for Yukon whiteite (Table II). Atomic coordinate parameters of jahnsite were used (Moore and Araki, 1974) and isomorphic replacement was applied. Cu-K_x radiation. 2. Yukon whiteite (analysis 2, Table III). 3. Taquaral whiteite. Ca-poor phase. 4. Taquaral whiteite. Type material. 5. Calculated powder pattern for jahnsite (type). Atomic coordinates from Moore and Araki (1974). Fe-K_a radiation. 6. Jahnsite (type). 7. Jahnsite (Fletcher pegmatite).

	I	2	3	4	5	6
$a(\text{\AA})$ $b(\text{\AA})$ $c(\text{\AA})$	14·90(4) 6·98(2) 10·13(2)	14:85(5) 6:92(4) 10:13(4)	14·99(2) 6·96(1) 10·14(1)	14·94(2) 7·14(1) 9·93(1)	15·01(3) 7·15(2) 9·87(2)	15 [.] 02 7 [.] 23
β	113° 07(10)'	112° 30(12)'	113° 19(6)'	110° 10(6)'	111° 14(10)'	_
c'(Å) β' $\rho(\text{obs, g cm}^{-3})$	18·64 91° 33' 2·58	18·72 91° 01′ —	18·63 91° 36' 2·67	18·65 88° 06' 2·71	18·42 88° 55' 2·86	18·75 — 2·85

TABLE II. Whiteites and jahnsites. Single-crystal data

I. Type white the from Taquaral. Single-crystal study and resulting cell parameters refined from powder data. Space group P_2/a .

2. Whiteite from Yukon. Cell parameters refined from powder data.

3. Ca-poor white ite from Taquaral. Single-crystal study and resulting cell parameters refined from powder data. Space group P_2/a .

4. Jahnsite (type). Data from Moore (1974). Space group $P_{2/a}$.

5. Jahnsite from the Fletcher mine. Single-crystal study and resulting cell parameters refined from powder data. Space group $P_{2/a}$.

6. Jahnsite from the Fletcher mine. Data from Mrose (1955). The space group was not stated.

	I		2	3	4	5	6		7		
	а	Ъ					а	b	a	Ъ	с
Na ₂ O	_		0.12	0.32	0.28		_		0.4	0.21	
CaŌ	6.0	6.7	5.98	3.80	3.57	I 4	6.6	6.9	2.6	3.27	_
MgO	10.2	10.6	12.55	11.32	9.99	10.1	9 [.] 4	9.9	2.7	3.39	
MnO	3.1	3.7	0.42	0.28	2.18	7.6	8.0	8.7	10.2	12.84	23.9
FeO	6.1	6.6	9.57	12.62	11.80	7.9			_	7.97	
Al_2O_3	12.0	13.2	11.24	I I·42	11.62	12.7	2·1	_	_	_	
Mn ₂ O ₃	_		-		_	_		—	_		
Fe ₂ O ₃	_	—	0.22	0.60	1.14	·	15.1	19.6	22.8	19.95	26.9
P_2O_5	36.0	37.5	37.68	36.86	37.49	36.4	32.2	35.0	29.6	33.12	31.9
$H_2O(-)$	- 1	01.4	10.32	9.76	5.92	- 1	18.8	1 10.0	- 1	19.00	1 7 7 - 2
$H_2O(+)$	- }	21.4	11.71	11.22	15.87	- }	10.0	19.9	- S	18.92	} I7·3
Total	73.7	100.0	99 [.] 75	99 [.] 53	99.86	76 [.] I	92.2	100.0	68.3	100.0	100.0

TABLE III. Whiteites and jahnsites. Chemical analyses*

* Unless otherwise stated, the formula unit is expressed as $XM(1)M(2)_2M(3)_2(H_2O)_8(OH)_2(PO_4)_4$.

1a. Type whiteite from Brazil. A. J. Irving, analyst.

Ib. Calculated composition for $X = Ca_{0.9}Mn_{0.1}^{2+}$; $M(I) = Fe_{0.7}^{2+}Mn_{0.3}^{2+}$; $M(2) = Mg_{1.0}$; $M(3) = Al_{1.0}$.

2. Yukon white ite. J. Ito, analyst. This yields $X = Ca_{0.81}Fe_{0.09}^{+}Mn_{0.05}^{2+}; M(1) = Fe_{0.92}^{+}Mg_{0.08}; M(2) = Mg_{1.00}; M(3) = Al_{0.85}Mg_{0.14}Fe_{0.14}^{+}Fe_{0.01}^{+}, Trace elements: K, Ba, Sr, Cr.$

3. Yukon white J. Ito, analyst. This yields $X = Ca_{0.53}Fe_{0.34}^2 Na_{0.08}Mn_{0.03}^{2+}; M(1) = Fe_{1.00}^{2+}; M(2) = Mg_{0.99}Fe_{0.01}^{2+}; M(3) = Al_{0.87}Mg_{0.10}Fe_{0.33}^{3+}$. Total includes 1.40 % SiO₂. Trace elements: Ba, Sr, Cr.

4. Yukon white ite. J. Ito, analyst. This yields $X = Ca_{0.49}Mn_{0.24}Fe_{0.09}^{2+}Na_{0.07}; M(1) = Fe_{1.00}^{2+}; M(2) = Mg_{0.90}Fe_{0.10}^{2+}; M(3) = Al_{0.88}Mg_{0.06}Fe_{0.06}^{2+}$. Trace elements: Zn, Ba, Sr, Cr.

5. Whiteite, Ca-poor variant from Brazil. J. Nelen, analyst. This yields $X = Mn_{0.8}^{2+}Ca_{0.2}; M(1) = Fe_{0.9}^{2+}Mn_{0.1}^{2+}; M(2) = Mg_{1.0}; M(3) = Al_{1.0}.$

6a. Type jahnsite from Moore (1974).

6b. Calculated composition for $X = Ca_{1.0}$; $M(1) = Mn_{1.0}^{2+}$; $M(2) = Mg_{1.0}$; $M(3) = Fe_{1.0}^{3+}$.

7a. Jahnsite from the Fletcher mine. A. J. Irving, analyst.

7b. Calculated composition for $X = Ca_{0.50}Mn_{0.36}^{2+}Na_{0.14}$; $M(I) = Mn_{1.00}^{2+}$; $M(2) = Fe_{0.48}^{2+}Mg_{0.36}Mn_{0.16}^{2+}Fe_{0.06}^{3+}$; $M(3) = Fe_{1.00}^{3+}$.

7c. Calculated composition for $Mn_3^{2+}Fe_3^{3+}(OH)_3(H_2O)_7(PO_4)_4$ (see Mrose, 1955).

Whiteite (type)	Whiteite (Ca-poor)	Jahnsite (type)*	Jahnsite (Fletcher)†
1.580(3)	1.575(5)	1.640(3)	1.682
1.585(3)	1.585(5)	1.658(3)	1.692
1.590(3)	1.595(5)	1.670(3)	1.707
+	-	_	-?
40-50°	80-90°	large	large
1.28	1.20	1.67	1.68
α∥b β∥a	$\alpha \bot \{001\}$	γ α:[001] 18	°
	(type) 1·580(3) 1·585(3) 1·590(3) + 40-50° 1·58 α b	(type) (Ca-poor) I·580(3) I·575(5) I·585(3) I·585(5) I·599(3) I·595(5) + - 40-50° 80-90° I·58 I·59 αb $\alpha \downarrow fool$	$\begin{array}{c ccccc} (type) & (Ca-poor) & (type)^* \\ \hline & & & \\ I^{+}580(3) & I^{+}575(5) & I^{+}640(3) \\ I^{+}585(3) & I^{+}585(5) & I^{+}658(3) \\ I^{+}590(3) & I^{+}595(5) & I^{+}670(3) \\ + & & & \\ 40^{-}50^{\circ} & 80^{-}90^{\circ} & large \\ I^{+}58 & I^{+}59 & I^{+}67 \\ \alpha \ b & \alpha + fool \\ \end{array}$

TABLE IV. Whiteite and jahnsite. Optical properties

* Moore (1974).

† Mrose (1955). The calculated mean index is based on analysis 7b in Table III.

‡ Calculated from the relationship of Gladstone and Dale, the cell contents, and specific gravities.

certain test for the species. Relative sizes of the dominant forms result in a variety of developments, the visual relationships of which are not immediately obvious. Fig. 2 presents several developments commonly found for jahnsites, which supplement the observations of Moore (1974*a*).

Mrose (1955), in a preliminary note, announced the occurrence of a '... yellow brown mineral occurring as crystals and sheaflike aggregates with rockbridgeite at the Fletcher and Palermo mines, New Hampshire ... ' and she suggests that this mineral '... resembles type xanthoxenite more closely than does the previously described xanthoxenite from Palermo'. She proposed the formula $Mn_3^{2+}Fe_3^{3+}(PO_4)_4(OH)_3.7H_2O$, although the details of the chemical analysis were not stated. Moore (1974*a*) alluded to the same material ('golden rockbridgeite' of New England collectors) in his paper.

The results of the powder and single-crystal studies on this material appear in Tables I and II respectively. It is quite clearly a variant of jahnsite group, and Mrose's single-crystal results can be related by noting that the twinned criteria derived from the primitive monoclinic cell closely match her orthogonal cell. Caution was taken to select a split fragment free from twinning; the hol and hil precession photographs clearly show the monoclinic aspect of the crystals. Results of an electronprobe analysis averaged from twelve grains appear in Table III under analysis 7a. Owing to the finely admixed nature of the material it was not possible to purify enough grains for wet chemical analysis. and, consequently, oxidation states have to be inferred. Like the whiteite samples from the type locality, the total is low. To derive the formula unit, the calculation was based on P = 4.00 such that the sum of the remaining cations leads to complete site occupancy.

We interpret the Fletcher material as a significantly oxidized transition metal-rich jahnsite. The balanced formula is

$$\begin{array}{c} Na_{0\cdot14}Ca_{0\cdot50}Mn_{1\cdot55}^{2\,+}Mg_{0\cdot72}Fe_{2\cdot14}^{3\,+}Fe_{0\cdot95}^{2\,+}\\ (OH)_{2\cdot00}(H_2O)_{8\cdot00}(PO_4)_{4\cdot00}. \end{array}$$

The proposed distributions of cations are:

It is practically impossible to distinguish among the possibility of vacancies in the X(I) position, the possible presence of hydronium cations, the partial hydroxylation of ligand water to balance charge, and the formal charges of the transition metals without a detailed structure analysis on the same crystals. Thus, the proposed distributions above are a compromise between the available analysis, the structure type, and the greater ease of Fe²⁺ oxidation relative to Mn²⁺. The good agreement between observed and calculated densities suggests that the above formula is probably a fair chemical

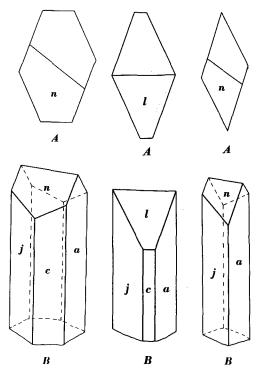


FIG. 2. Crystals of jahnsite showing the forms $c\{001\}$, $a\{100\}$, $j\{\overline{2}01\}$, $l\{011\}$, and $n\{\overline{1}11\}$. A. Plan. B. Clinographic projection (b-axis polar). *Left*: Tip Top pegmatite, South Dakota. *Centre*: Sapucaia pegmatite, Minas Gerais, Brazil. *Right*: Palermo No. 1 pegmatite, New Hampshire.

description of Fletcher material. The end-member is jahnsite— $(CaMn^{2+}Fe^{2+})$.

It is proposed that the general composition of the jahnsite series be written jahnsite—(XM(I)M(2))and the whiteite series whiteite—(XM(I)M(2)). Thus, type jahnsite is jahnsite— $(CaMn^{2+}Mg)$; the Fletcher material, jahnsite— $(CaMn^{2+}Fe^{2+})$; type whiteite and the Yukon samples, whiteite— $(CaFe^{2+}Mg)$; and the Ca-poor variant, whiteite— $(Mn^{2+}Fe^{2+}Mg)$. End-member compositions, adhering to convention, accept the dominant cation at each site.

This classification parallels that for the pumpellyite and julgoldite series proposed by Passaglia and Gottardi (1973) where two kinds of octahedral positions, X (predominantly divalent cations) and Y (predominantly trivalent cations) are involved. The series is split first on the basis of Y populations— Al^{3+} for pumpellyite, Fe^{3+} for julgoldite—and then by the predominant cation in X. Thus, with $X = Fe^{2+}$ and $Y = Al^{3+}$, the nomenclature is pumpellyite— (Fe^{2+}) . It is appealing to split the series this way since the electrostatic bond strengths for Al^{3+} and Fe^{3+} are considerably greater than those of X-population cations in pumpellyitejulgoldite and the XM(1)M(2) positions and cations in white ite-jahnsite.

The whiteite-jahnsite series is complicated by the presence of three distinct octahedral positions and uncertainties necessarily arise with regard to site distributions. In principle, chemical composition and refined crystal structure must be known for each crystal in order to assure a reasonably correct assignment of cations over the X, M(1), and M(2)positions. This is clearly a difficult task and we propose that tentative distributions of cations proceed from ionic radii arguments where the radius increases M(3) < M(2) < M(1) < X. Thus, once the composition is known, the contents are calculated on the basis of the formula XM(1) $M(2)_2 M(3)_2^{3+}(OH)_2(H_2O)_8[PO_4]_4$ and the smallest trivalent cations are placed in M(3) until that site is filled, then M(2), etc., until the largest remaining cations are placed in X. It is possible, in oxidized and leached variants, that X may be only partly occupied or empty.

New data on xanthoxenite

A review of xanthoxen and xanthoxenite. Xanthoxenite is an enigmatic species. Originally described by Laubmann and Steinmetz (1920) as Xanthoxen from the Hühnerkobel pegmatite, Bavaria, Frondel (1949) resurrected the name for a basic calcium ferric phosphate from the Palermo No. 1 mine, North Groton, New Hampshire. This conclusion was reached, despite inconsistencies between the original description and his results, on the basis of the identity of a sample labelled 'xanthoxenite' from Hühnerkobel with the Palermo material. A complete wet-chemical analysis on the Palermo material led Frondel (1949) to propose the formula $Ca_2Fe^{3+}(PO_4)_2(OH)$. $I_2^{+}H_2O$. Unfortunately, Frondel could not locate the type specimen of Laubmann and Steinmetz. He stated, 'The conclusion thus seems forced that the Palermo material is identical with xanthoxenite, in spite of the discrepancies in the description of the two substances.'

It was impossible to locate any 'xanthoxenite' or 'xanthoxen' sample that unambiguously proved to be the type specimen and we must depend on the descriptive data of Laubmann and Steinmetz (1920). They remarked that the crystals are thin tabular parallel to {010}, monoclinic, the cleavage perfect parallel to {010} and that the mineral is frequently in parallel growth with needles of *Kakoxen* (= cacoxenite). These needles of 'cacoxenite' were observed to extinguish at 8° from the prism axis. This suggests that their 'cacoxenite' is probably strunzite since γ :[001] ranges from 10 to 19° in that mineral according to Frondel (1957), whereas true cacoxenite is hexagonal and would exhibit parallel extinction.

The crucial information rests on fig. 20 of Laubmann and Steinmetz (1920) and the attendant discussion, the former reproduced as fig. 3 in the present investigation. It represents morphological and optical data based on their microscopic study of the type 'xanthoxenite' crystals. Parallel to the plane of the perfect {010} cleavage, the clinodome was observed to make a 41° angle with the outline of the prism. In addition, the γ optic direction provided an acute angle of 36° with the outline of the prism. Mrose (1955) proposed that the yellowbrown material (the jahnsite of the present study) occurring as crystals and sheaf-like aggregates from the Fletcher mine is closer to the material of Laubmann and Steinmetz than the materials of

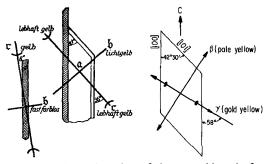


FIG. 3. Optical orientation of the acute bisectrix for stewartites resting on their $\{010\}_m$ cleavage surfaces. *Left*: Fig. 20 of Laubmann and Steinmetz (1920). *Right*: Sketched data of Tennyson (1956).

Frondel. Since jahnsite possesses good cleavage parallel to $\{001\}$ and since [010] is the prism direction, the relationship between the Fletcher and the Hühnerkobel materials is not easily reconciled. In addition, jahnsite crystals are nearly always flattened parallel to $\{100\}$ or $\{\overline{2}01\}$, lie on these surfaces, and extinguish parallel to [010]. Finally, tabular development parallel to $\{001\}$ of the kind found for whiteite would provide an acute interior angle of about 50° .

The identity of 'xanthoxenite' was a puzzle until the monoclinic data of Tennyson (1956) on stewartite were examined. Peacor (1963) has shown that stewartite actually possesses a triclinic pseudomonoclinic cell. The pseudo-monoclinic (m) cell of Tennyson (1956) is related to the triclinic (t) cell as follows: $a_m = c_t$; $b_m = 2a_t + 6b_t - c_t$, $c_m = a_t$ according to Peacor (1963). Based on the Peacor cell, Moore and Araki (1975) solved the stewartite crystal structure with the refined parameters a 10.398 Å, b 10.672 Å, c 7.223 Å, α 90.10°, β 109·10°, γ 71·83°. Tennyson (1956) reported $a_{\rm m}$ 7.17 Å, $b_{\rm m}$ 60.8 Å, $c_{\rm m}$ 10.41 Å, β 109° 32', specific gravity 2.466, hardness 3, all b 1.612 (almost colourless), β : [001] 32° 1.653 (pale yellow), γ : [001] 58° 1.681 (gold yellow). In addition, she described the Hagendorf crystals as thin tabular parallel to $\{010\}_m$, most frequently showing the bounding zones [001]_m and [101]. On the basis of the structure analysis of Moore and Araki (1974b), the plane of perfect cleavage is nearly parallel to the $\{010\}_m$ plane since it is parallel to the strongly bonded octahedral and tetrahedral sheets and cuts only weak bonds between these sheets. Reconstruction of the optical and X-ray data of Tennyson (1956) in fig. 3 yields the angle 42° 30' between the [100] and [101] bounding zones, the pleochroism and orientation of the indicatrix arranged similar to that featured in Laubmann and Steinmetz (1920) except for a widened y: [001] 58° angle. The cleavage, interior angles, and the orientation of the indicatrix all provide strong evidence that the 'xanthoxen' of Laubmann and Steinmetz (1920) is in fact stewartite. Since stewartite has chronological priority (Schaller, 1912), the name 'xanthoxen' is a synonym.

Do the remaining data of Laubmann and Steinmetz (1920) agree with stewartite? More recent observations reveal that the contact between crystals of stewartite and strunzite is frequently observed whereas the association between strunzite and jahnsite is of rare occurrence. In fact, the stewartite, strunzite, pseudolaueite, and laucite polymorphs often occur together. The reported specific gravity of 2.844 by Laubmann and Steinmetz (1920) is unusually high for stewartite but this is probably based on the separate from the 'Kraurit' (= rockbridgeite) intergrowths. Finally, they report $32.61\% P_2O_5$ and $16.1\% H_2O$ (by ignition). Stewartite, $Mn^{2+}Fe_2^{3+}(OH)_2(H_2O)_6$ [PO₄]₂.2H₂O ideally has $26.6\% P_2O_5$ and 26.9%H₂O.

To resolve this conflict we submit the following interpretation, based on the Fletcher mine paragenesis and a description by Laubmann and Steinmetz (1920). At Fletcher, the orange phase that replaces the rockbridgeite and occurs in intimate 'intergrowth' with it is invariably jahnsite but the small yellow crystals in open cavities of the same prove to be stewartite with variable amounts of laueite and strunzite. Laubmann and Steinmetz (1920) state, 'Es ist entweder in Strahlig blätterigen Aggregaten mit dem Kraurit verwachsen oder hat sich in kleinen Kryställchen von gypsähnlichen Form in dessen Hohlräumen vielfach neben wirrstrahligen Kakoxen abgeschieden.' Thus, their paragenesis almost exactly duplicates our observations on Fletcher material. It is likely, from the two observations above, that their optical and morphological data pertain to stewartite and that the specific gravity and partial chemical analysis correspond to the earlier-formed jahnsite, which occurs in intimate contact with rockbridgeite. This proposition is appealing since the cavity minerals probably formed by partial hydrothermal attack on the rockbridgeite and jahnsite and reflect the higher water content and lower P2O5 content of a later lowtemperature cavity paragenesis. The distinction among the minerals jahnsite, stewartite, laueite, and pseudolaueite-in the absence of an X-ray study-is a perplexing task in descriptive mineralogy.

Xanthoxenite as species. We propose that the xanthoxenite of Frondel (1949) be adopted as the specific term in mineralogical nomenclature and that his material be defined as the neotype. It is a late-stage mineral and occurs as a cavity and fracture filling from the Palermo pegmatite, Hühner-kobel, Hagendorf, numerous pegmatites in the Black Hills of South Dakota, and from Přibyslavice and Otov, Czechoslovakia. Associated minerals include laueite, strunzite, stewartite, mitridatite, siderite, etc.

Professor F. Cěch kindly provided specimens of 'xanthoxen' from Přibyslavice and Otov; some of these proved to be jahnsite, others the xanthoxenite of Frondel (1949). The two phases can be visually distinguished by the more brittle and transparent character of jahnsite and the very soft, waxy translucent and pulverulent character of the latter mineral. One specimen of the xanthoxenite from Přibyslavice afforded a small single crystal for detailed study (examination of many Palermo specimens failed to provide a suitable crystal). Owing to a mosaic spread of 3° and relatively few strong reflections, the single-crystal data from rotation, Weissenberg, and precession photographs about the principal zones are of mediocre quality: triclinic, a 6.70(4)Å, b 8.85(4)Å, c 6.54(3)Å, $\alpha 92.1(2)^{\circ}$, $\beta 110.1(2)^{\circ}$, $\gamma 93.2(2)^{\circ}$, Z = 1 for the formula $Ca_4Fe_2^{3+}(OH)_2(H_2O)_3[PO_4]_4$. The cleavage is $\{010\}$ perfect. The calculated density is 3.38g cm⁻³ for the ideal formula, considerably higher than the specific gravity of 2.97 reported by Frondel (1949) on Palermo Mine material. A Gladstone-Dale calculation using the specific refractive energies for CaO, P2O5, and H2O in Larsen and Berman (1934) and k = 0.274 for Fe₂O₃ proposed by Moore (1974b); and the mean index of $\langle n \rangle =$ 1.714 from Frondel (1949) yields 3.06 gm cm^{-3} . Substituting cations of lower atomic number and the friable nature of the material will contribute to lower specific gravity than that of the pure salt. Knowledge of the crystal structure is desirable, a study that is presently in progress.

About 0.2 g of Přibyslavice material was handpicked for a wet-chemical analysis. The small amount of brown stain easily dissolved in a weak acid solution. The complete analysis (Table V) affords results similar to those reported by Frondel (1949). Both analyses agree well with the formula $Ca_4Fe_2^{3+}(OH)_2(H_2O)_3[PO_4]_4$. The excess water reported may be either adsorbed or the result of a weak occupancy in the structure. Frondel (1949) published an optical orientation and a crystal outline of the Palermo material parallel to the {010} plane. He discerned two principal planes on the microscopic crystals making an acute angle of 34°. We note that the transformation of our cell to c' = c - a affords an acute angle a [100]:c' $[001]' = 34^{\circ} 23'.$

Partly indexed powder data for the Přibyslavice xanthoxenite appear in Table VI. The agreement with the results of Frondel (1949) is excellent and leaves little doubt that the two materials are identical.

A further remark on the xanthoxenite problem. The foregoing manuscript, excepting the recently studied Yukon material, was completed in January 1975 and communicated to the International Commission on New Minerals and New Mineral Names. Shortly thereafter, Mrs. Kay Robertson of Los Angeles, California, U.S.A., a micromounter who specializes in Hagendorf phosphates, brought to our attention a paper by H. Strunz (1971), who reached the same conclusion that fig. 20 of Laubmann and Steinmetz (1920) is in fact stewartite. Mrs. Robertson added, in a personal communication, that the type specimens of Laubmann and Steinmetz, housed in Munich State Collection, were destroyed during World War II. A more

recent paper by Strunz, Forster, and Tennyson (1975), however, not only overlooks reference to the earlier conclusion, but asserts that jahnsite and xanthoxenite are synonymous! They state 'Xanthoxen wurde ursprünglich von Laubmann und Steinmetz (1920) als neues Mineral vom Hühnerkobel beschrieben, allerdings waren für die optischen Daten offentsichtlich irrtümlich Stewartit-Kristalle verwendet worden.' They continue: 'Dabei zeigte es sich, dass die mit "Xanthoxen" etikettierten Stufen z.T. tatsächlich Stewartit enthielten, zum anderen Teil in sehr geringen Mengen ein schlecht ausgebildetes braunes Mineral, den echten Xanthoxen [italics ours]. Laubmann and Steinmetz, however, based their description on the crystals shown herein to be in accord with the properties of stewartite and made no mention of material that fits the description of Strunz et al. We are forced to conclude that the recent contribution to the xanthoxenite problem is without any scientific foundation.

Salmonsite discredited: a mixture of hureaulite and jahnsite

During February 1976 Mrs. Robertson brought our attention to another paper, a note by Sobott (1973), who proposed that a new secondary phosphate from Hagendorf may in fact be salmonsite or a salmonsite-related phase. Schaller (1912), in the original description of the species from the Stewart mine, Pala, California, proposed the formula $Fe_2O_3.9MnO.4P_2O_5.14H_2O$ $Mn_9^{2+}Fe_2^{3+}$ or (PO₄)₈.14H₂O. This species for long intrigued us but persistent search for single-crystal material always met with failure. Upon examining the Sobott paper, we were struck by the similarity between a photomicrograph of a Hagendorf crystal aggregate with that of jahnsite. These crystals show characteristic tabular-prismatic development with striations parallel to {010} and consist of clearly identifiable $a\{100\}, j\{\overline{2}01\}, and$ $n{III}$, much resembling the development of type crystals. Sobott compared powder photographs of two samples, his nos. 7992 and 8117, with the data for salmonsite, published in part by Fisher (1958) and listed complete in the ASTM File 13-337. Although a fair agreement occurs between some of the lines of the Hagendorf material with those of salmonsite, substantial differences, especially with respect to missing lines in the Hagendorf samples, exist.

We re-examined salmonsite, the specimen used by Fisher in his study, since efforts to locate Schaller's type material proved fruitless. Fortunately, Schaller's description was sufficient to establish with confidence that the Pala sample

	Ι	2	3	4		5	6
Na ₂ O	0.10	0.10		0.01)		—)	
K ₂ O	0.02	0.02		-			
CaO	28·0	29.3	24.99	1.95 {	2·01	1.68	20.2
MgO	o [.] 48	0.20	0.91	0.05 (2.01	0.08 2.00	30.3
SrO	0.11	0.11	_	- 1			
MnO	-		4.22	_)		0·24)	
Al ₂ O ₃	0.55	0.23		0.02		-)	
Fe_2O_3	15.9	16.6	21.68	o•78 }	0.99	1.02 } 1.02	21.6
Mn_2O_3	3.94	4.10	_	0.19)	
P_2O_5	36.2	38.1	37.62	2.00		2.0	38.4
H ₂ O (200 °C)	1.12	1.17	o∙86	0.48		0.36	
H ₂ O (1100 °Ć)	9 [.] 34	9.73	9.13	4.03	4.21	3.83 4.19	9.2
SiO ₂ (insol.)	3.90	_	0.28	_			
CO ₂	absent		_	_			
Total	99.89	100.0	100.23				100.0

TABLE V. Xanthoxenite. Chemical analyses

1. Přibyslavice, Czechoslovakia. Jun Ito, analyst.

2. Recomputed after deducting insol.

3. Palermo Mine, N. Groton, New Hampshire. Hallowell analysis in Frondel (1949).

4. Cations based on P = 2 for (2). 5. Cations based on P = 2 for (3). 6. Ca₄Fe₂³⁺(OH)₂(H₂O)₃[PO₄]₄.

This s	tudy							Frond	lel (1949)		
I/I ₀	d _{obs}	$d_{\rm calc}$	hkl	I/I ₀	$d_{\rm obs}$	d_{calc}	hkl	I/I_0	d _{obs}	I/I ₀	$d_{ m obs}$
80	6.272	6.270	100	10	2.401	2.396	112	50	6.24	10	2.36
30	4.935	4.897		10	2.313	2.323	222	40	4.94	20	2.30
90	3.489	3.489	120	30	2.235	2.234	131	70	3.48	60	2.23
40	3.341	3.372	III	20	2.093	2.090	300	_		10	2.08
70	3.236	3.232	Ī02	10	2.013	2.016	013	80	3.22	10	2.01
70	3.136	3.134	200	_		_		20	3.12	10	1.84
100	3.055	3.063	002	10	1.725	1.726	033	100	3.02	20	1.72
40	2.973	2.988	121	-		-		10	2.96	10	1.65
50	2.741	2.714	2 02	—		-		90	2.73	10	1.57
—		2.714	03Ī	20	1.231			_		30	1.53
40	2.688	2.648	220	15	1.465	_	_	20	2.68	10	1.44
30	2.619	2.591	031	_	-	_				10	1.41
30	2.611	2.602	212	_		-	_	40	2.60	10	1-36
30	2.464	2·47 I	220	_		_	_	20	2.46	10	1.30

TABLE VI. Xanthoxenite. Powder data*

* This study: Cu- K_{α} radiation, graphite monochromator, chart speed 1° min⁻¹ in 2 θ , Si (5·4301 Å) internal. Miller indices are based on strong single crystal reflections. Sample in this study from Přibyslavice, Czechoslovakia; sample of Frondel (1949) from Palermo mine, New Hampshire, U.S.A.

I			2		3		4		5	
I/I_0	d _{calc}	hkl	I/I_0	d _{obs}	I/I_0	d_{obs}	I/I ₀	dobs	I/I_0	$d_{\rm obs}$
		_	100	9 [.] 42 J	90	9·26 J	vs	9·70 J	vs	9 [.] 54 J
59	8.737	200	30	8.83 H	45	8·68 H		-	—	_
89	8.061	110	70	8·12 H	50	8·04 H	W	7.92 ?	—	_
_			—		_	-	m	7.02 J	—	_
16	6.271	III	10	6·33 H			m	6·16 J?		_
16	5.947	111	10	5.99 H	10	5.957 H		_	—	_
_			10	5.75 J	15	5.687 J			w	5.81 ?
_		-	50	5.03 J	50	5.005 J	m	5·10 J	S	5.03 J
-			-	— —	20	4 [.] 893 J		— 	_	
26	4.670	002	60	4·70 H+J	75	4.659 H+J	m	4·78 J	s	4.71 J
32	4.528	311	20	4.22 H	25	4·529 H			—	_
-		_	10	4.39 ?			m	4.32 ?		
13	4.085	021	20	4·09 H+J	25	4.092 J	_	_	m	4·14 J
18	4.031	220			10	4.040 H	_	—		
_		_	20	3·962 J	20	3·936 J			m	3·97 J
12	3.631	221	20	3·804 ?		 3·588 Н			_	_
-			10	3.648 H	20				_	
		-	50	3·525 J	65	3·527 J	w	3.22	s	3·54 J
			_		45	3·500 J	_	<u> </u>		
20	3.256	022	30	3·276 H+J	20	3·275 H+J		—	w	3·32 J
25	3.228	312	_	_	25	3·243 H	_		_	—
26	3.189	511	_	-	35	3.185 H + J	_	_		
100	3.136	<u>2</u> 22	100	3·160 H	85	3·149 H+J	_	_	w	3·15 J
20	3.063	421	10	3·069 H	20	3.065 H	8	3.07 ?	_	—
17	3.020	402			25	3·036 H	—	_		—
10	2.980	511			_			_	_	
62	2.973	222	80	2·990 H+J	55	2.987 H+J	—	—	W	2·91 J
19	2.912	600	_	_	35	2·912 H	_	_	—	—
-			—		20	2·874 J		-	—	
10	2.853	113	100	2·853 H+J	100	2·842 H+J	vs	2·88 J	vs	2·88 J
11	2.718	4 22		-			m	2.70 ?		
32	2.620	<u>3</u> 31	50	2·62 H	10	2·629 H	m	2.61 J	m	2·61 J
11	2.611	602		_	45	2.606 H+J		—	—	
13	2.568	023	10	2·564 H+J	10	2·556 H+J			—	_
11	2.546	331	5	2.51 H					_	_
16	2.431	621	30	2.444 H	10	2.431 H	-		—	—
7 8	2.397	711	20	2.405 H	10	2·398 H	_	—		
10	2.335	004 6 a t	30	2·363 H+J	35	2·367 H+J	m	2·36 J	m	2·36 J
8	2·316 2·289	621 530	10	2·327 H+J	 I0				_	_
7	2·289 2·270	530 711	10	2·279 H		2·270 H	_		_	_
7	2·270 2·264	622	_						_	_
8	2·204 2·244	022 712	_		_			_		
14	2·244 2·184	800		2·19 H	10	2·186 H	_	_		
16	2·184 2·176	ī33	10	2.19 H 2.148 H		2.180 H	_	_		
5	2.170	423		2 140 II	_					_
5	2.127	423 332	_	_	_			_	_	_
7	2.090	332 333	10	2·098 H	_		_	_	_	
6	2.090	555 224	10	2.056 H+J	_	-	_	_	_	_
9	2.033	314	20	2.03 H+J	10	2·026 H+J			m	2·03 J
		440				II J				5

TABLE VII. Salmonsite powder data compared with hureaulite (H) and jahnsite $(J)^*$

* To assess jahnsite (J) contribution, compare with column 5 in Table I.

Hureaulite. Calculated powder pattern. Cu-K_α radiation.
 Salmonsite. ASTM File 13-337.
 Salmonsite. This study. Graphite monochromator, Cu-K_α radiation, ¹/₂° min⁻¹.
 Sobott (1973). Sample 7992.
 Sobott (1973). Sample 8117.

	I	2	3	4	5	6
CaO	1.06	1.06	2.31	_	_	1.77
MnO	37.74	20.74	45.22	48 ∙66	31.91	40.87
FeO	0.13	0.13	0.28	_		7.48
Fe_2O_3	9.53	0.00	_	-	17.96	0.16
P_2O_5	34.86	17.89	39.00	38.98	31.92	39.02
H_2O^+	15.30	5.62	12.25	12.36	18.21	10.43
H ₂ O	0.43	0.43	0.94	_	_	_
Insol.	1.40	0.00		—		0.89
	100.45	45 [.] 87	100.00	100.00	100.00	100.62

TABLE VIII. Salmonsite. Interpretation of chemical analysis

1. Analysis of salmonsite in Schaller (1912).

2. After deduction of 5322% $Mn_2^{2+}Fe^{3+}(OH)(H_2O)_4(PO_4)_2$ (jahnsite— $Mn^{2+}Mn^{2+}Mn^{2+})$ and 1.4% insoluble.

3. Column 2 renormalized to 100%. 4. Pure $Mn_3^{2+}(H_2O)_4(PO_3(OH))_2(PO_4)_2$ (hureaulite).

5. Pure Mn_2^2 + Fe³⁺(OH)(H₂O)₄(PO₄)₂ (jahnsite -- MnMnMn).

6. 'Palaite' (= hureaulite) in Schaller (1912).

studied by Fisher and us is in fact salmonsite ('It results from the partial oxidation and hydration of hureaulite, and forms cleavable masses of a buff color . . .'). A diffractometer trace on the buffcoloured massive material confirmed the powder pattern previously reported by Fisher. A calculated powder pattern for hureaulite was retrieved from the structure-analytical results of Moore and Araki (1973), and the same from the structure of type jahnsite as reported by Moore and Araki (1974). These results, the salmonsite patterns and the patterns of Sobott for Hagendorf material are listed in Table VII. Calculated powder patterns are reliable means of checking observed powder data since the former are free from the bias of impurities, preferred orientation effects, and sample shape.

Table VII reveals that salmonsite is in fact a mixture of hureaulite and jahnsite, although a minor amount of some impurity is present. The samples of Sobott are more difficult to ascertain owing to obvious differences between the two. The match between strong intensities is adequate but, owing to significant differences resulting from substitutions encountered among powder patterns for members of the jahnsite structure type, the final arbiter must rest on single-crystal study. Here, Sobott's material is tentatively identified as belonging to the jahnsite structure type.

Is the salmonsite used in this study equivalent to the type material? Many scientists in the past have been deceived through investigations on specimens other than types. This is not surprising in light of the close crystal-chemical relations among the basic phosphates of iron and manganese, especially laueite, pseudolaueite, stewartite, whitmoreite, jahnsite, and xanthoxenite. Strong additional evidence does exist, however, to establish salmonsite

as a true mixture and not a discrete homogeneous phase. In Table VIII, the chemical analysis of salmonsite by Schaller (1912) is reproduced. Structural evidence indicates that hureaulite does not tolerate Fe³⁺, so all Fe₂O₃ reported was assumed to belong to the jahnsite phase. Since FeO is minor and MgO is absent, it is assumed that the jahnsite fraction has composition $Mn_2^{2+}Fe^{3+}(OH)$ $(H_2O)_4(PO_4)_2$, i.e. jahnsite-Mn²⁺Mn²⁺Mn²⁺. Deducting 53.2% of the total composition as jahnsite and 1.4% as insoluble, the remainder is assumed to be hureaulite. Renormalizing to 100% reveals an excellent agreement with the ideal hureaulite composition. It may be protested the CaO belongs to the jahnsite phase, but that would not alter the conclusion: on grounds of the powder pattern and chemical analysis, salmonsite is a mixture of approximately equal amounts of hureaulite and jahnsite. The original analysis of Schaller deviates greatly from that of either hureaulite or jahnsite so it was not possible to infer a relationship to these species in earlier studies.

Let us finally remark that optical properties of salmonsite, hureaulite, and jahnsite do not afford good determinative tools. In Table IX the indices overlap and, furthermore, the birefringences are similar. Even the pleochroism is not a reliable guide. Perhaps the most significant distinguishing character is the orientation of the γ vibration direction: in jahnsite this is parallel to the prism (= [010]) but in hureaulite it is inclined by 75° from the prism axis (= [001]). The two reported sources for complete optical data on salmonsite are in conflict with respect to dispersion. We could not resolve this conflict in our sample owing to the extremely small grain size of the individuals.

We are forced to conclude that the original salmonsite of Schaller was in fact a mixture of two phases in about equal amount, namely hureaulite and jahnsite, and the name should be abandoned. Salmonsite is, thus, a breakdown product derived from the oxidation and aquation of hureaulite. This is supported by the analysis in Schaller (1912) for 'palaite' = hureaulite, listed in Table VIII. Grouping CaO with MnO, an equation can be written:

 $(Mn_{0.85}Fe_{0.15})_{5}^{2+}(H_{2}O)_{4}[PO_{3}OH]_{2}[PO_{4}]_{2}+$ $1.12H_2O + 0.41O_2 \rightarrow$ 'palaite' (= hureaulite) $0.55Mn_5(H_2O)_4[PO_3OH]_2[PO_4]_2 +$ hureaulite $0.75 Mn_2^2 + Fe^{3+}(OH)(H_2O)_4[PO_4]_2 + 0.30 PO_4^{3-}$ jahnsite

This equation is a typical example of aquation and oxidation of the pre-existing phase so typical of phosphate formation in pegmatites at low temperature. The recrystallized hureaulite is essentially a pure phase. Hureaulite coexisting with jahnsite is common, occurring at the Fletcher, Palermo, and Tip Top pegmatites, and it is evident that the stability fields of these two phases overlap to some degree.

Conclusions

The two species whiteite and jahnsite are defined on the basis of the structure type and the formal composition $XM(1)M(2)_2M(3)_2(OH)_2(H_2O)_8$ [PO₄]₄ and are named whiteite—(XM(1)M(2))for $M(3) = Al^{3+} > Fe^{3+}$ and jahnsite—(XM(1)M(2)) for Fe³⁺ > Al³⁺. Established approaches to end-member compositions include whiteite—(CaFe²⁺Mg) (type), whiteite— $(Mn^{2+}Fe^{2+}$ Mg), jahnsite—(CaMn²⁺Mg) (type), jahnsite —(CaMn²⁺Fe²⁺) (Fletcher), and possibly jahnsite— $(Mn^{2+}Mn^{2+})$ (Pala). Correct establishment of end-member composition may require formal structure analysis for some materials.

The xanthoxenite of Frondel is established as the nominate species, having probable composition $Ca_4Fe_2^{3+}(OH)_2(H_2O)_3[PO_4]_4$. The original xanthoxenite of Laubmann and Steinmetz was most likely stewartite.

Salmonsite is a fine-grained intimate mixture of hureaulite and jahnsite in about equal proportions and, therefore, is not deserving of specific status. In outline:

```
Established species:

whiteite—(XM(I)M(2)), this study.

jahnsite—(XM(I)M(2)), Moore (1974a, b),

this study.

xanthoxenite, Frondel (1949).

Discredited species:

'xanthoxenite' = stewartite (in part), Laub-

mann and Steinmetz (1920).

'salmonsite' = hureaulite + jahnsite,

Schaller (1912).
```

These three nomenclatural problems were each submitted separately to the International Commission on New Minerals and New Mineral Names (IMA) and they received approval. Samples used in this study will be deposited in the U.S. National Museum of Natural History (Smithsonian Institution).

Acknowledgements. Mrs. Kay Robertson, a most diligent and determined person, offered continued inspiration and assistance throughout this study. Without her help, neither the salmonsite nor the xanthoxenite problems would have received the detailed attention so necessary in nomenclatural revisions.

Independent electron-probe analyses by Dr. A. J. Irving (on the University of Chicago facility) and Mr. J. Nelen (U.S. National Museum) presented special problems owing to the complex chemistry, water content, and physical properties of the grains and their efforts are appreciated. Dr. R. V. Gaines donated a fine sample of the

	1 Salmonsite	2 Jahnsite (type)	3 Jahnsite (Fletcher)	4 Hureaulite
α	1.655	1.640	1.682	1.647
β	1.66	1.658	1.692	1.654
γ	1.670	1.670	1.707	1.660
2V	very large	large	?	75°
Sign Pleochroism:	+	_	— ?	_
α	nearly colourless	pale purple	pale yellow-brown	colourless
β	?	deep purplish brown	vellow-brown	vellow to pale rose
γ	orange-yellow	yellow (green tinge)	dark yellow-brown	reddish yellow to reddish brown
Dispersion Orientation	r < v strong γ elongation	? ? prism (= [010])	r > v strong ?	r < v very strong $\gamma:[001] 75^{\circ}$

TABLE IX. Salmonsite. Summary of optical data

I. Larsen and Berman (1934). Palache *et al.* give essentially the same results except that β is yellow and r > v strong. Schaller (1912) states, 'Mean refractive index about 1.66, double refraction low. In thin section yellow and non-pleochroic.'

2. Moore (1974) on crystals from Tip Top pegmatite, Custer, South Dakota.

3. Mrose (1955).

4. Larsen and Berman (1934).

Ca-poor variant for further study. Mr. A. R. Kampf assisted in the optical determinations and Mr. D. H. Lund prepared the crystal drawings.

This study was supported by the NSF Grant GA-40543 and the Sloan Foundation Grant-in-Aid BR-1489.

REFERENCES

- Fisher (D. J.), 1958. Am. Mineral. 43, 181-207.
- Frondel (C.), 1949. Ibid. 34, 692-705.
- —— 1957. Neues Jahrb. Mineral. Monatsh. 222–6.
- Larsen (E. S.) and Berman (H.), 1934. U.S. Geol. Surv. Bull. 848, 30-2.
- Laubmann (H.) and Steinmetz (H.), 1920. Z. Kristallogr. Mineral. 55, 523-85.
- Mandarino (J. A.) and Sturman (B. D.), 1976. Can. Mineral. 14, 127-31.

- Moore (P. B.), 1974a. Am. Mineral. 59, 48-59.
- —— Araki (T.), 1973. Am. Mineral. 58, 302-7.
- ——— 1974a. Ibid. **59**, 964-73.
- ——— 1974b. Ibid. 1272-6.
- Mrose (M. E.), 1955. Geol. Soc. Am. Progr. and Abstr. 1955 Meetings, 76A.
- Palache (C.), Berman (H.), and Frondel (C.), 1951. Dana's System of Mineralogy, 2.
- Passaglia (E.) and Gottardi (G.), 1973. Can. Mineral. 12, 219-23.
- Peacor (D. R.), 1963. Am. Mineral. 48, 913-14.
- Schaller (W. T.), 1912. J. Wash. Acad. Sci. 2, 143-5.
- Sobott (R.), 1973. Der Aufschluss, 233-5.
- Strunz (H.), 1971. Ibid. 72-4.
- ----- Forster (A.), and Tennyson (Ch.), 1975. Ibid. 175-7.
- Tennyson (Ch.), 1956. Naturwiss. 43, 128-9.
- [Manuscript received 5 April 1977]