JAHNSITE-(NaMnMg), A NEW JAHNSITE-GROUP MINERAL FROM THE SAPUCAIA MINE, BRAZIL AND THE WHITE ROCK NO. 2 QUARRY, AUSTRALIA

Anthony R. Kampf[§]

*Mineral Sciences Department, Natural History Museum of Los Angeles County, 900 Exposition Boulevard,
Los Angeles, California 90007, USA*

Peter Elliott

*Department of Earth Sciences, School of Physical Sciences, The University of Adelaide, Adelaide,
South Australia 5005, Australia*
South Australian Museum, North Terrace, Adelaide, South Australia 5000, Australia

Barbara P. Nash

Department of Geology and Geophysics, University of Utah, Salt Lake City, Utah 84112, USA

Luigi Chiappino

via Palmanova 67, I-20132 Milano, Italy

Sergio Varvello

via Vincenzo de Vit 17, I-28838 Stresa, Italy

Abstract

Jahnsite-(NaMnMg), $(Na,Ca)(Mn^{2+},Fe^{3+})(Mg,Fe^{3+},Mn^{3+})_2Fe^{3+}_2(PO_4)_4(OH)_2(H_2O)_8$, is a new mineral from the Sapucaia pegmatite, Conselheiro Pena pegmatite district, Minas Gerais, Brazil, and the White Rock No. 2 quarry, Bimbowrie Conservation Park, South Australia, Australia. At both localities, it is a low temperature, secondary mineral formed as the result of alteration of primary phosphates. The mineral occurs as light orange to orange-yellow prisms, elongate on [100], exhibiting the forms {100}, {001}, and {011} and twinned by reflection on {001}. The streak is white, the luster is vitreous, and crystals are transparent to translucent. The Mohs hardness is about 4. The tenacity is brittle, the fracture is irregular, stepped (splintery), and there is one very good cleavage on {001}. The measured density is 2.68(1) g/cm^3 (Sapucaia). The mineral is slowly soluble in dilute HCl. Jahnsite-(NaMnMg) from Sapucaia is biaxial (–), with α 1.642(1), β 1.675(1), γ 1.677(1) (white light). The measured 2*V* is 29(1)°. Dispersion is very strong, *r* < *v*. The optical orientation is *Z* = **b**; *X* ^ **c** = 51° in obtuse β. Pleochroism is *X* = colorless, *Y* and *Z* = orange-yellow; *Y* ≈ *Z* > *X*. Electron-microprobe analyses gave the empirical formulae $(Na_{0.56}Ca_{0.25}Mn^{2+}_{0.09})_{\Sigma0.90}(Mn^{2+}_{0.85}Fe^{3+}_{0.15})_{\Sigma1.00}(Mg_{1.53}Fe^{3+}_{0.47})_{\Sigma2.00}(Fe^{3+}_{1.79}Al_{0.21})_{\Sigma2}(PO_4)_4(OH)_{1.83}(H_2O)_{8.17}$ for the Sapucaia material and $(Na_{0.63}Ca_{0.23}Mn^{2+}_{0.14})_{\Sigma1.00}(Mn^{2+}_{0.68}Mn^{3+}_{0.26}Fe^{3+}_{0.05}Mg_{0.01})_{\Sigma1.00}(Mg_{1.26}Mn^{2+}_{0.43}Mn^{3+}_{0.16}Fe^{3+}_{0.15})_{\Sigma2.00}(Fe^{3+}_{1.97}Al_{0.02})_{\Sigma1.99}(PO_4)_4(OH)_{1.98}(H_2O)_{8.02}$ for the White Rock material. The mineral is monoclinic, space group *P2/a*, with cell parameters (Sapucaia) *a* 15.1045(15), *b* 7.1629(2), *c* 9.8949(7) Å, β 110.640(7)°, *V* 1001.83(13) Å^3, and *Z* = 2. The structure refinements of crystals from both localities were generally consistent and showed the mineral to be a member of the jahnsite group (Sapucaia: R_1 = 3.19% for 1941 I_o > 2σ*I* reflections; White Rock: R_1 = 6.94% for 13485 I_o > 2σ*I* reflections).

Keywords: jahnsite-(NaMnMg), new mineral, jahnsite group, crystal structure, electron microprobe analysis, Sapucaia mine, Brazil, White Rock No. 2 quarry, Australia.

§ *Corresponding author e-mail address*: akampf@nhm.org

INTRODUCTION

The jahnsite group (Table 1) was recently formally approved by the Commission on New Minerals Nomenclature and Classification (CNMNC) of the International Mineralogical Association (IMA) (Kampf *et al*. 2018a). Members of this group have the general formula $XM1M2_2M3_2(H_2O)_8(OH)_2(PO_4)_4$, where the X site accommodates the largest cations, the $M1$ and $M2$ sites accommodate medium- to small-sized octahedrally coordinated cations (*e.g.*, Mn^{2+}, Fe^{2+}, Fe^{3+}, and Mg^{2+}), and the $M3$ site accommodates the small octahedrally coordinated cations Fe^{3+} or Al^{3+}. This formula was originally given by Moore & Ito (1978), who proposed a naming scheme in which the root name jahnsite is applied to minerals with $M3 = Fe^{3+}$ and whiteite to those with $M3 = Al^{3+}$; the root name is then followed by a suffix of the form -($XM1M2$). In the newly approved group nomenclature, the group is subdivided into the jahnsite subgroup (where $M3 = Fe^{3+}$) and the whiteite subgroup (where $M3 = Al^{3+}$).

The name of the new jahnsite-group mineral described herein, jahnsite-(NaMnMg), is in accord with the aforementioned naming scheme. The jahnsite root name signifies that the M3 site is occupied dominantly by Fe^{3+} and the suffix is based upon the dominance of Na at the X site, Mn at the $M1$ site, and Mg at the $M2$ site. The new mineral and name have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA 2018-017; Kampf *et al*. 2018b). The holotype specimen from the Sapucaia mine is housed in the collections of the Mineral Sciences Department, Natural History Museum of Los Angeles County, 900 Exposition Boulevard, Los Angeles, California 90007, USA, catalogue number 66701. The cotype specimen from the White Rock No. 2 quarry is deposited in the collections of the South Australian Museum, North Terrace, Adelaide, South Australia, Australia, registration number G34298.

OCCURRENCE AND PARAGENESIS

Jahnsite-(NaMnMg) has been found at two localities. The holotype specimen was collected in 2010 by one of the authors (SV) on the dumps of the Sapucaia pegmatite (18°54′2″S, 41°29′4″W), about 12 km NNE of Galiléia, Conselheiro Pena pegmatite district, Minas Gerais, Brazil. The cotype specimen was collected in 1993 from the White Rock No. 2 quarry (32°4′53″S, 140°19′45″E), situated in the Bimbowrie Conservation

TABLE 1. MEMBERS OF THE JAHNSITE GROUP*

Name	X	M1	M2[§]	M3[§]	Reference
			Site assignments		
Jahnsite subgroup					
Jahnsite-(CaMnMg)	Ca^{2+}	Mn^{2+}	Mg^{2+}	Fe^{3+}	Moore (1974); Moore & Araki (1974)
Jahnsite-(CaMnFe)	Ca^{2+}	Mn^{2+}	Fe^{2+}	Fe^{3+}	Moore & Ito (1978)
Jahnsite-(MnMnMn)	Mn^{2+}	Mn^{2+}	Mn^{2+}	Fe^{3+}	Moore & Ito (1978)
Jahnsite-(CaMnMn)	Ca^{2+}	Mn^{2+}	Mn^{2+}	Fe^{3+}	Grice *et al*. (1990)
Jahnsite-(NaFeMg)	Na^+	Fe^{3+}	Mg^{2+}	Fe^{3+}	Kampf *et al*. (2008)
Keckite	Ca^{2+}	Mn^{2+}	Fe^{3+}	Fe^{3+}	Hochleitner & Fehr (2010)
Jahnsite-(CaFeMg)	Ca^{2+}	Fe^{2+}	Mg^{2+}	Fe^{3+}	Elliott (2016a)
Jahnsite-(MnMnMg)	Mn^{2+}	Mn^{2+}	Mg^{2+}	Fe^{3+}	Vignola *et al*. (2018)
Jahnsite-(MnMnZn)	Mn^{2+}	Mn^{2+}	Zn^{2+}	Fe^{3+}	Kampf *et al*. (2018a)
Jahnsite-(NaMnMg)	Na^+	Mn^{2+}	Mg^{2+}	Fe^{3+}	This study
Whiteite subgroup					
Whiteite-(MnFeMg)	Mn^{2+}	Fe^{2+}	Mg^{2+}	Al^{3+}	Moore & Ito (1978)
Whiteite-(CaFeMg)	Ca^{2+}	Fe^{2+}	Mg^{2+}	Al^{3+}	Moore & Ito (1978); Capitelli *et al*. (2011)
Whiteite-(CaMnMg)	Ca^{2+}	Mn^{2+}	Mg^{2+}	Al^{3+}	Grice *et al*. (1989)
Rittmannite	Mn^{2+}	Mn^{2+}	Fe^{2+}	Al^{3+}	Marzoni Fecia Di Cossato *et al*. (1989)
Whiteite-(CaMnMn)	Ca^{2+}	Mn^{2+}	Mn^{2+}	Al^{3+}	Grey *et al*. (2010); Yakovenchuk *et al*. (2012)
Whiteite-(CaMgMg)	Ca^{2+}	Mg^{2+}	Mg^{2+}	Al^{3+}	Kampf *et al*. (2016)
Whiteite-(MnMnMg)	Mn^{2+}	Mn^{2+}	Mg^{2+}	Al^{3+}	Elliott (2016b)

* Several species mentioned in the literature, but never approved by the IMA, are not included.
[§] The $M2$ and $M3$ sites in the general formula each correspond to two similar structural sites, $M2a/M2b$ and $M3a/M3b$, respectively.

Fig. 1. Jahnsite-(NaMnMg) crystals coating partially altered blades of albite from the Sapucaia mine. The black botryoidal material is rockbridgeite. The field of view is 7 mm across.

Park, about 22 km N of Olary, South Australia, Australia.

The Sapucaia pegmatite is a zoned pegmatite that has been mined since the 1920s for various commercial minerals (*e.g.*, muscovite, beryl, feldspar), but is best known mineralogically for its complex phosphate mineral assemblages (see Baijot *et al*. 2012, and references therein). Jahnsite-(NaMnMg) was found in vugs in matrix consisting mostly of frondelite and albite in association with meurigite-K (K slightly dominant over Na), phosphosiderite, and strengite. Jahnsite-(NaMnMg) crystals are found growing directly on surficially altered albite blades (Fig. 1), which presumably are the source of the Na. Baijot *et al*. (2012) discussed two triphylite alteration sequences at Sapucaia leading to two different secondary phosphate mineral assemblages. Assemblage I involves oxidizing conditions, while Assemblage II does not. Baijot *et al*. (2012) noted that jahnsite-series (jahnsite group, jahnsite subgroup) phases occur in Assemblage I, consistent with the presence of essential Fe^{3+} in jahnsites. By contrast, they noted that whiteite-series (jahnsite-group, whiteite-subgroup) phases occur in assemblage II, consistent with the presence of Al in place of Fe^{3+} in the structure.

The White Rock pegmatite is one of more than 70 pegmatite bodies in the Olary Province of South Australia (Lottermoser & Lu 1997). The pegmatite is characterized as belonging to the beryl-columbite-phosphate-rare element type in the classification of Černý (1991). Three quarries, White Rock Nos. 1, 2, and 3, have been excavated from the White Rock pegmatite to recover feldspar (both albite and microcline) and beryl. Feldspar production from 1932 to 1958 is estimated to have been 1213 tonnes.

The pegmatite is mineralogically zoned, characterized by the occurrence of late-stage phosphate nodules between the quartz core and intermediate feldspar-rich zone (Lottermoser & Lu 1997). Jahnsite-(NaMnMg) occurs here in seams in a matrix comprising triplite, fluorapatite, and quartz. Associated minerals are phosphosiderite, ushkovite, strunzite, and bermanite. The triplite–zwieselite was formed by metasomatic alteration of magmatic fluorapatite and has been transformed by hydrothermal alteration and weathering, in an oxidizing, low-temperature, low-pH environment, to produce a complex, microcrystalline intergrowth of secondary phosphate minerals (Lottermoser & Lu 1997). On the cotype specimen, ushkovite and phosphosiderite are the earliest-formed minerals. Bermanite and strunzite overgrow ushkovite and phosphosiderite, and jahnsite-(NaMnMg) overgrows ushkovite. The presence of bermanite, in particular, indicates a very oxidizing environment and is consistent with some of the Mn in jahnsite-(NaMnMg) from the White Rock occurrence being Mn^{3+}, consistent with the empirical formula presented below.

The jahnsites from Sapucaia studied by Baijot *et al*. (2012) all belonged to solid solutions between jahnsite-(MnMnMg) and jahnsite-(CaMnMg). Sodium is a minor constituent in the jahnsites from Sapucaia studied by Baijot *et al*. (2012) and, indeed, Na is at most only a minor constituent in the vast majority of jahnsites worldwide. The only other approved jahnsite species with essential Na is jahnsite-(NaFeMg), first described from the Tip Top pegmatite, South Dakota, USA (Kampf *et al*. 2008) and later reported from the Angarf-Sud pegmatite, Morocco (Kampf *et al*. 2012) and from Tom's quarry, South Australia (Elliott *et al*. 2014). Jahnsite-(NaMnMg) was previously reported from the Tip Top pegmatite by Kampf *et al*. (2008), forming small zones in crystals that were mostly jahnsite-(NaFeMg); however, the limited extent of these zones did not permit the full characterization of the species.

PHYSICAL AND OPTICAL PROPERTIES

At both localities, jahnsite-(NaMnMg) occurs as light orange to orange-yellow prisms, elongate on [100]. Prisms from the Sapucaia mine are up to 0.5 mm long (Fig. 2), while those from the White Rock No. 2 quarry are only up to 0.06 mm long (Fig. 3). Crystals exhibit the forms {100}, {001}, and {011}, and they are ubiquitously twinned by reflection on {001} (Fig. 4). The streak is very pale yellow, the luster is vitreous, and crystals are transparent. No fluorescence was observed under SW or LW ultraviolet radiation. The Mohs hardness is about 4. The
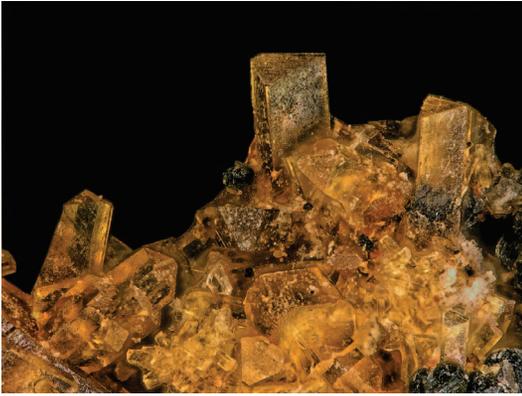
Fig. 2. Twinned jahnsite-(NaMnMg) prisms with black rockbridgeite from the Sapucaia mine. The field of view is 0.84 mm across.

tenacity is brittle, the fracture is irregular and stepped (splintery), and there is one perfect cleavage on {001}. The density of a Sapucaia crystal measured by flotation in methylene iodide – toluene is 2.68(1) g/cm^3 and that of a White Rock crystal measured in an aqueous solution of sodium polytungstate is 2.69(3) g/cm^3; the calculated densities based on the empirical formulae are 2.684 and 2.738 g/cm^3, respectively. At room temperature, the mineral is slowly soluble in dilute HCl.

The optical properties measured from a crystal from Sapucaia in white light show the mineral to be biaxial (–) with $\alpha = 1.642(1)$, $\beta = 1.675(1)$, $\gamma = 1.677(1)$. The $2V$ measured directly with a spindle stage is $27(2)°$ and using extinction data analyzed with the program EXCALIBR (Gunter *et al.* 2004) is $29(1)°$; the calculated $2V$ is $27.2°$. Dispersion is very
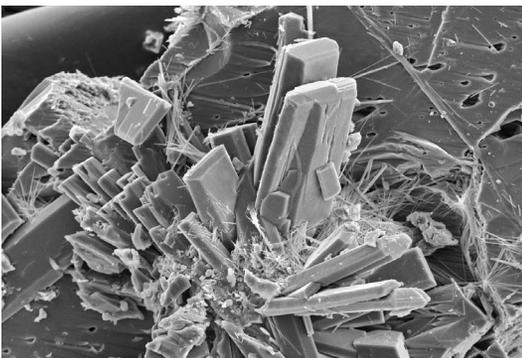

Fig. 3. SEM image of jahnsite-(NaMnMg) blades from White Rock No. 2 quarry. The blades are up to 40 μm in length.
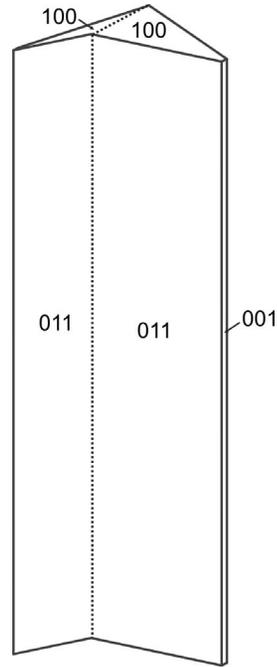

Fig. 4. Drawing of a twinned jahnsite-(NaMnMg) crystal; clinographic projection in non-standard orientation, {100} vertical. The twin plane is shown by dotted lines.

strong, $r < v$. Pleochroism is $X =$ colorless, Y and $Z =$ orange-yellow; $Y \approx Z > X$. The optical orientation is $Z = \mathbf{b}$; $X \wedge \mathbf{c} = 51°$ in obtuse β.

CHEMICAL COMPOSITION

Chemical analyses of Sapucaia material (14 spots on five crystals) were obtained using a Cameca SX-50 electron microprobe in the Department of Geology and Geophysics at the University of Utah (WDS mode, 15 kV, 20 nA, 10 μm beam diameter) utilizing Probe for EPMA software. Chemical analyses of White Rock material (24 spots on two crystals) were acquired using a Cameca SXFive electron microprobe at the University of Adelaide (WDS mode, 15 kV, 20 nA, 5 μm beam diameter). Raw X-ray intensities were corrected for matrix effects with a $\phi(\rho z)$ algorithm (Pouchou & Pichoir 1991). There was insufficient material for CHN analyses; consequently, we calculated H_2O on the basis of P = 4, charge balance, and 26 O *apfu*, as determined by the crystal structure analysis (see below). Analytical data are given in Table 2.

The empirical formulae based on 26 O *apfu* and formatted in accord with the structure refinements and informed by the OccQP site occupancy analyses are $(Na_{0.56}Ca_{0.25}Mn^{2+}_{0.09})_{\Sigma0.90}(Mn^{2+}_{0.85}Fe^{3+}_{0.15})_{\Sigma1.00}$

TABLE 2. ANALYTICAL DATA (wt.%) FOR JAHNSITE-(NaMnMg)

Constituent	Sapucaia mine[a]			White Rock No. 2 quarry[b]		
	Mean	Range	SD	Mean	Range	SD
Na_2O	2.16	1.74–2.45	0.21	2.35	1.19–3.51	0.59
CaO	1.73	1.31–2.21	0.27	1.53	0.72–4.89	0.95
MgO	7.64	7.21–7.91	0.22	6.15	5.41–6.92	0.42
MnO^c	8.27	7.49–10.07	0.81	10.72	7.25–15.92	2.43
$Mn_2O_3^c$	–	–	–	3.94	5.41–6.92	0.03
Fe_2O_3	23.83	22.39–25.12	0.79	20.77	18.10–23.79	1.83
Al_2O_3	1.31	0.77–1.84	0.29	0.13	0.03–0.27	0.08
P_2O_5	35.23	34.71–35.70	0.29	34.02	32.44–35.22	0.74
H_2O^d	20.31			19.45		
Total	100.48			99.06		

[a] Standards: albite (Na, Al), diopside (Ca, Mg), rhodonite (Mn), hematite (Fe), and apatite (P).
[b] Standards: albite (Na), plagioclase (Ca), almandine–pyrope (Al, Fe, Mg), rhodonite (Mn), and fluorapatite (P).
[c] MnO and Mn_2O_3 are apportioned based on the structural site occupants calculated using OccQP, which provides $Mn^{2+}_{0.752}Mn^{3+}_{0.248}$.
[d] Based on the structure.

$(Mg_{1.53}Fe^{3+}_{0.47})_{\Sigma 2.00}(Fe^{3+}_{1.79}Al_{0.21})_{\Sigma 2}(PO_4)_4(OH)_{1.83}$ $(H_2O)_{8.17}$ for Sapucaia material and $(Na_{0.63}Ca_{0.23}$ $Mn^{2+}_{0.14})_{\Sigma 1.00}(Mn^{2+}_{0.68}Mn^{3+}_{0.26}Fe^{3+}_{0.05}Mg_{0.01})_{\Sigma 1.00}$ $(Mg_{1.26}Mn^{2+}_{0.43}Mn^{3+}_{0.16}Fe^{3+}_{0.15})_{\Sigma 2.00}(Fe^{3+}_{1.97}Al_{0.02})_{\Sigma 1.99}$ $(PO_4)_4(OH)_{1.98}(H_2O)_{8.02}$ for White Rock material. Note that the White Rock empirical formula corresponds almost exactly to the OccQP results because that calculation was strongly weighted toward the EPMA results (see below).

The endmember formula for jahnsite-(NaMnMg), $NaMn^{2+}Mg_2Fe_2(PO_4)_4(OH)_2(H_2O)_8$, is not charge balanced. Charge balance is attained by Ca and Mn^{2+} substituting at the X site and Fe^{3+} and/or Mn^{3+} substituting at the $M1$ and $M2$ sites. Note that the structure refinements coupled with site occupancy analyses using OccQP (see below) indicate that all Fe in material from both localities is 3+, while Mn is all 2+ in Sapucaia material and both 2+ and 3+ in White Rock material.

The Gladstone-Dale compatibility index (Mandarino 2007) $1 - (K_P/K_C)$ is 0.007 (superior) for Sapucaia material.

X-ray Crystallography and Crystal Structure Refinement

Both powder and single-crystal X-ray studies of holotype material from the Sapucaia mine were done using a Rigaku R-Axis Rapid II curved imaging plate microdiffractometer with monochromatized $MoK\alpha$ radiation. A polycrystalline sample was used for the powder-diffraction study; a Gandolfi-like motion on the φ and ω axes was used to further randomize the

sample. Observed d values and intensities were derived by profile fitting using JADE 2010 software (Materials Data, Inc.). Data are given in Table 3. Unit-cell parameters refined from the powder data using JADE 2010 with whole pattern fitting are a 15.096(4), b 7.153(4), c 9.888(74) Å, β 110.575(8)°, and V 999.6(7) Å^3.

An untwinned crystal fragment was used for the structure refinement. The Rigaku CrystalClear software package was used to process the structure data, including the application of an empirical multi-scan absorption correction using ABSCOR (Higashi 2001). SHELXL-2013 (Sheldrick 2015) was used to refine the structure. The starting atom coordinates for the structure refinement were taken from the structure determination of jahnsite-(NaFeMg) by Kampf et al. (2008). The occupancies of the cation sites were refined and the cation-site scattering values from the refinement were used with the program OccQP (Wright et al. 2001) to analyze the likely site populations (see below). The OccQP-calculated cation site populations were then used in the final refinement. Difference Fourier syntheses located all H atom sites, which were then refined with soft restraints of 0.82(3) Å on the O–H distances and 1.30(3) Å on the H–H distances, and with the U_{eq} of each H atom tied to that of its O atom (×1.5 for OH and ×1.2 for H_2O). Details of the data collection and structure refinement are provided in Table 4, fractional coordinates and atom displacement parameters in Table 5, cation-site scattering values and OccQP calculated site populations in Table 6, selected interatomic distances and angles in Table 7, and bond valences in Table 8.

TABLE 3. POWDER X-RAY DIFFRACTION DATA (*d* IN Å) FOR JAHNSITE-(NaMnMg) FROM SAPUCAIA

I_{obs}	d_{obs}	d_{calc}	I_{calc}	h k l	I_{obs}	d_{obs}	d_{calc}	I_{calc}	h k l
100	9.29	9.2598	100	0 0 1	9	2.0565	2.0638	2	3 3 $\bar{2}$
8	7.11	7.1629	3	0 1 0			2.0505	2	1 3 2
		7.0675	3	2 0 0			2.0341	2	5 2 1
4	6.39	6.3894	4	1 1 0	19	2.0098	2.0089	10	4 2 2
14	5.69	5.7006	9	1 1 $\bar{1}$			2.0013	3	4 0 3
		5.6656	3	0 1 1	16	1.9669	1.9726	4	6 1 $\bar{4}$
27	5.02	5.0309	18	2 1 0			1.9670	9	4 2 $\bar{4}$
		4.9751	3	2 1 $\bar{1}$	33	1.9436	1.9476	4	2 3 2
30	4.91	4.9062	23	1 1 1			1.9465	4	4 0 $\bar{5}$
		4.7075	2	2 0 $\bar{2}$			1.9442	16	0 2 4
19	4.65	4.6299	18	0 0 2			1.9273	2	2 1 4
4	4.075	4.0698	6	1 1 $\bar{2}$			1.9059	2	3 1 $\bar{5}$
20	3.935	3.9364	17	3 1 0	22	1.8874	1.8871	17	8 0 $\bar{2}$
32	3.546	3.5608	12	3 1 $\bar{2}$			1.8605	2	8 0 $\bar{1}$
		3.5338	18	4 0 0	6	1.8293	1.8211	3	1 3 3
		3.4939	2	1 1 2	15	1.7875	1.7907	10	0 4 0
18	3.462	3.4577	16	4 0 $\bar{2}$			1.7669	2	8 0 0
6	3.336	3.3403	4	0 2 1			1.7592	2	1 4 $\bar{1}$
16	3.294	3.2905	11	3 1 1	8	1.7487	1.7470	4	4 2 3
		3.2850	2	2 0 $\bar{3}$			1.7289	3	8 0 $\bar{4}$
13	3.181	3.1947	4	2 2 0	7	1.7190	1.7176	2	2 3 $\bar{4}$
		3.1803	4	2 2 $\bar{1}$			1.7103	3	4 2 $\bar{5}$
		3.1691	2	4 1 0	8	1.6731	1.6702	3	0 4 2
		3.1620	2	1 2 1	4	1.6397	1.6354	2	3 3 3
		3.0470	3	2 1 2	7	1.5951	1.5973	4	4 4 0
26	2.975	2.9710	25	4 0 1			1.5901	3	4 4 $\bar{2}$
20	2.878	2.8818	17	4 0 $\bar{3}$	19	1.5850	1.5845	12	8 2 0
		2.8745	8	3 1 $\bar{3}$	10	1.5542	1.5569	7	8 2 $\bar{4}$
91	2.834	2.8328	81	0 2 2	8	1.5367	1.5433	5	0 0 6
		2.6296	3	5 1 0			1.5337	5	4 4 1
33	2.601	2.5980	25	4 2 $\bar{1}$	14	1.5235	1.5235	8	4 2 4
4	2.507	2.5154	3	4 2 0			1.5210	3	4 4 $\bar{3}$
		2.4876	2	4 2 $\bar{2}$	13	1.4894	1.4930	8	4 2 $\bar{6}$
6	2.423	2.4266	2	4 0 2			1.4855	3	8 0 2
		2.4128	2	1 2 $\bar{3}$	6	1.4495	1.4409	3	4 4 2
20	2.352	2.3635	4	6 6 $\bar{1}$			1.4252	2	4 4 $\bar{4}$
		2.3537	5	4 0 $\bar{4}$	4	1.4180	1.4164	2	0 4 4
		2.3460	6	6 1 $\bar{2}$	5	1.3761	1.3722	4	8 2 2
		2.3381	2	0 2 3	6	1.3382	1.3395	3	4 2 5
6	2.301	2.2969	2	1 1 $\bar{4}$			1.3368	4	8 2 $\bar{6}$
		2.0733	2	1 1 4					

Only calculated lines with intensities ≥2 are included.

TABLE 4. DATA COLLECTION AND STRUCTURE REFINEMENT DETAILS FOR
JAHNSITE-(NaMnMg) FROM SAPUCAIA

Diffractometer	Rigaku R-Axis Rapid II
X-ray radiation/power	MoKα ($\lambda = 0.71075$ Å)/50 kV, 40 mA
Temperature	293(2) K
Space group	$P2/a$
Unit-cell dimensions	$a = 15.1045(15)$ Å
	$b = 7.1629(2)$ Å
	$c = 9.8949(7)$ Å
	$\beta = 110.640(7)°$
V	1001.83(13) Å^3
Z	2
Density (for structural formula)	2.700 g·cm^{-3}
Absorption coefficient	2.929 mm^{-1}
$F(000)$	812.9
Crystal size	$120 \times 120 \times 70$ µm
θ range	3.19 to 27.47°
Index ranges	$-19 \le h \le 19, -9 \le k \le 7, -12 \le l \le 12$
Reflections collected/unique	9016/2276 [$R_{int} = 0.036$]
Reflections with $I_o > 2\sigma I$	1941
Completeness to q = 27.47°	99.0%
Refinement method	Full-matrix least-squares on F^2
Parameters refined/restraints	196/13
GoF	1.081
Final R indices ($I_o > 2\sigma I$)	$R_1 = 0.0319$, w$R_2 = 0.0720$
R indices (all data)	$R_1 = 0.0391$, w$R_2 = 0.0757$
Largest diff. peak/hole	$+0.91/-0.49$ e/A^3

* $R_{int} = \Sigma|F_o^2 - F_o^2(\text{mean})|/\Sigma[F_o^2]$. GoF = $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$. $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. w$R_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$. $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where a is 0.0375, b is 0.6106, and P is $[2F_c^2 + \text{Max}(F_o^2,0)]/3$.

Tables of observed and calculated structure factors are available from the Depository of Unpublished data on the Mineralogical Association of Canada website [document jahnsite-(NaMnMg), CM56, 18-00053][1].

Structure data were also collected for cotype jahnsite-(NaMnMg) from the White Rock quarry. Because of the small size of the twinned crystal, data were collected using synchrotron X-ray radiation ($\lambda = 0.71080$ Å). The resulting refinement was consistent with that for the holotype; however, largely because of the twinning, the refinement was not as good and complete results are only reported for the holotype. Nevertheless, the structure refinement for the cotype yielded site scattering factors and bond distances that were analyzed using OccQP to elucidate the cation assignments in the empirical formula (Table 6). The cell parameters for the White Rock cotype are a 15.096(5), b 7.1600(14), c 9.925(2) Å, and β 110.84(3)°

Structure Description

Jahnsite-(NaMnMg) is isostructural with other members of the jahnsite group, which have the general formula $XM1M2_2M3_2(PO_4)_4(OH)_2 \cdot 8H_2O$. The X site has eight-fold coordination and hosts the largest cations in the structure. The M sites all have six-fold octahedral coordination and generally rank in size as follows: $M1 > M2 > M3$. The $M2$ and $M3$ sites each correspond to two nonequivalent, but structurally similar, sites, $M2a/M2b$ and $M3a/M3b$, respectively. The structure is based on a chain of $M3O_4(OH)_2$ octahedra linked by sharing *trans*-OH corners with one another and further linked by sharing corners of PO_4 tetrahedra decorating the chains. The structure possesses dense slabs of $[XM1M3_2(OH)_2(PO_4)_4]^{4-}$ oriented parallel to {001}, which are bridged by PO_4 corner-sharing to $M2O_2(H_2O)_4$ octahedra (Fig. 5). The H-atom positions have been determined for several jahnsite-group species [jahnsite-(NaFeMg), jahnsite-

[1] The MAC website can be found at http://mineralogicalassociation.ca

TABLE 5. ATOM COORDINATES AND DISPLACEMENT PARAMETERS ($Å^2$)
FOR JAHNSITE-(NaMnMg) FROM SAPUCAIA

	x/a	y/b	z/c	U_{eq}
X	0.25	0.97021(14)	0	0.0264(2)
M1	0.25	0.47232(7)	0	0.01254(13)
M2a	0.5	0	0.5	0.0174(2)
M2b	0.25	0.50365(12)	0.5	0.0140(2)
M3a	0	0	0	0.01090(13)
M3b	0	0.5	0	0.01133(13)
P1	0.18573(4)	0.26411(8)	0.18734(7)	0.01379(15)
P2	0.08097(4)	0.74458(8)	0.79732(7)	0.01281(15)
O1	0.27677(14)	0.2399(3)	0.1503(2)	0.0296(5)
O2	0.20817(14)	0.3055(3)	0.3443(2)	0.0243(4)
O3	0.12452(13)	0.0910(2)	0.1425(2)	0.0272(4)
O4	0.13985(11)	0.4343(2)	0.08528(19)	0.0174(4)
O5	0.18557(12)	0.6787(3)	0.8580(2)	0.0241(4)
O6	0.05501(13)	0.7822(2)	0.6377(2)	0.0214(4)
O7	0.07671(13)	0.9239(2)	0.87932(19)	0.0218(4)
O8	0.01684(12)	0.5929(2)	0.82168(19)	0.0201(4)
OH	0.02733(13)	0.7508(2)	0.0972(2)	0.0174(4)
H	0.000(2)	0.752(4)	0.151(3)	0.026
OW1	0.22565(17)	0.7237(3)	0.3433(2)	0.0307(5)
H1A	0.258(2)	0.726(4)	0.292(3)	0.037
H1B	0.1705(18)	0.746(4)	0.271(3)	0.037
OW2	0.44911(17)	0.2141(3)	0.3462(2)	0.0349(5)
H2A	0.473(2)	0.232(5)	0.284(4)	0.042
H2B	0.3926(17)	0.214(4)	0.283(3)	0.042
OW3	0.62887(16)	0.9899(3)	0.4598(3)	0.0350(5)
H3A	0.655(3)	1.007(5)	0.541(3)	0.042
H3B	0.643(2)	0.914(4)	0.420(3)	0.042
OW4	0.39097(15)	0.5131(3)	0.5159(2)	0.0265(5)
H4A	0.405(2)	0.591(4)	0.478(3)	0.032
H4B	0.425(2)	0.477(4)	0.587(3)	0.032

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
X	0.0260(6)	0.0173(5)	0.0278(6)	0	-0.0005(5)	0
M1	0.0114(3)	0.0130(3)	0.0140(3)	0	0.0055(2)	0
M2a	0.0179(4)	0.0147(4)	0.0168(5)	−0.0042(3)	0.0027(4)	0.0000(3)
M2b	0.0142(5)	0.0147(4)	0.0133(5)	0	0.0050(4)	0
M3a	0.0108(2)	0.0080(3)	0.0133(3)	−0.00082(17)	0.0036(2)	−0.00013(16)
M3b	0.0108(2)	0.0092(3)	0.0149(3)	−0.00010(17)	0.0057(2)	−0.00015(16)
P1	0.0117(3)	0.0151(3)	0.0134(3)	−0.0021(2)	0.0030(2)	0.0008(2)
P2	0.0123(3)	0.0136(3)	0.0129(3)	0.0008(2)	0.0049(2)	0.0014(2)
O1	0.0188(10)	0.0477(13)	0.0225(11)	0.0049(8)	0.0074(8)	0.0134(8)
O2	0.0320(11)	0.0239(10)	0.0159(10)	−0.0031(8)	0.0070(8)	0.0004(8)
O3	0.0252(10)	0.0172(9)	0.0272(11)	0.0013(8)	-0.0057(8)	−0.0017(7)
O4	0.0116(8)	0.0162(9)	0.0233(9)	−0.0010(7)	0.0047(7)	0.0004(6)
O5	0.0148(9)	0.0329(11)	0.0232(10)	0.0017(8)	0.0050(8)	0.0071(8)
O6	0.0274(10)	0.0193(9)	0.0159(9)	0.0027(7)	0.0056(8)	0.0012(7)
O7	0.0281(10)	0.0168(9)	0.0269(10)	−0.0022(7)	0.0177(8)	−0.0024(7)
O8	0.0230(9)	0.0182(9)	0.0219(10)	0.0003(7)	0.0114(8)	−0.0020(7)
OH	0.0204(10)	0.0125(9)	0.0204(10)	−0.0007(7)	0.0086(8)	0.0006(6)
OW1	0.0380(13)	0.0306(11)	0.0286(12)	0.0068(9)	0.0182(10)	0.0091(9)
OW2	0.0364(13)	0.0302(11)	0.0249(12)	0.0034(9)	−0.0057(10)	−0.0055(10)
OW3	0.0332(13)	0.0315(13)	0.0440(14)	−0.0124(10)	0.0183(11)	−0.0026(9)
OW4	0.0199(10)	0.0268(11)	0.0327(13)	0.0094(8)	0.0093(9)	−0.0012(8)

TABLE 6. CATION SITE OCCUPANCIES AND SITE SCATTERING VALUES FOR JAHNSITE-(NaMnMg)

| Site | Site Scattering Values* | | OccQP calculated site populations |
	Refinement	OccQP	
Sapucaia mine			
X	31.3	31.3	$Na_{0.569}Ca_{0.277}Mn^{2+}_{0.154}$
$M1$	50.1	49.6	$Mn^{2+}_{0.601}Fe^{3+}_{0.375}Mg_{0.024}$
$M2a$	31.8	31.8	$Mg_{0.712}Mn^{2+}_{0.151}Fe^{3+}_{0.137}$
$M2b$	27.7	27.7	$Mg_{0.809}Fe^{3+}_{0.106}Mn^{2+}_{0.055}\square_{0.030}$
$M3a$	49.3	49.3	$Fe^{3+}_{0.896}Al_{0.104}$
$M3b$	50.5	50.4	$Fe^{3+}_{0.940}Al_{0.060}$
White Rock No. 2 quarry			
X	32.8	30.4	$Na_{0.622}Ca_{0.224}Mn^{2+}_{0.154}$
$M1$	50.1	49.7	$Mn^{2+}_{0.684}Mn^{3+}_{0.260}Fe^{3+}_{0.049}Mg_{0.007}$
$M2a$	34.8	34.6	$Mg_{0.592}Mn^{2+}_{0.249}Mn^{3+}_{0.159}$
$M2b$	33.1	33.0	$Mg_{0.666}Mn^{2+}_{0.182}Fe^{3+}_{0.152}$
$M3a$	49.7	51.0	$Fe^{3+}_{0.971}Al_{0.018}\square_{0.011}$
$M3b$	50.4	51.7	$Fe^{3+}_{0.994}\square_{0.006}$

* Site scattering value = mean atomic number × site multiplicity.

(MnMnMg), whiteite-(CaMgMg), and whiteite-(Ca-FeMg); see Table 1 for references].

The hydrogen bond scheme for jahnsite-(NaMnMg) is almost the same as that for other jahnsite-group structures with determined H positions. The one difference is the OW2–H2a···OH hydrogen bond in jahnsite-(NaMnMg) instead of a OW2–H2a···OW4 bond as seen in the other structures. It should be noted, however, that the H2a site in jahnsite-(NaMnMg) is only about 1.5 Å from the H site (of the OH group), and that the hydrogen bonds from OH to OW2 and from OW2 to OH virtually coincide, but in opposite directions. A refinement of the occupancies of the H and H2a sites indicated them to be approximately half occupied, consistent with ½ hydrogen bond in each direction; however, we do not believe that the quality of the data warrants definitively drawing that conclusion. The unusual location of the H2a site could be an artefact of the data.

CATION SITE OCCUPANCIES

Moore & Ito (1978) recommended that "tentative distributions of cations proceed from ionic radii arguments where the radius increases $M3 < M2 < M1 < X$". This approach is generally applied in defining all jahnsite-group minerals for which structure refinements are not possible. Nevertheless, whenever possible, it is recommended that structure refinements be employed for determining the cation-site occupants and, thereby, for defining the species. Complex cation compositions, which sometimes involve possible mixed cation valences, require special

care and the consideration of composition, charge balance, site scattering, and bond valence. For this purpose, the program OccQP (Wright et al. 2001) is particularly useful. This program uses quadratic equations in a constrained least-squares formulation to optimize occupancy assignments based upon site scattering, chemical composition, charge balance, bond valence, and cation–anion bond lengths.

The assignment of cations to the sites in the jahnsite-(NaMnMg) structure is complicated because of the presence of six cations, Na^+, Ca^{2+}, Mn^{2+}, Fe^{3+}, Mg^{2+}, and Al^{3+}, in the crystals from the Sapucaia mine and seven, Na^+, Ca^{2+}, Mn^{2+}, Mn^{3+}, Fe^{3+}, Mg^{2+}, and Al^{3+}, in the crystals from the White Rock quarry. The apportionment of Mn as Mn^{2+} and Mn^{3+} in the White Rock crystals was assessed as part of the OccQP analysis. For both calculations, the following constraints were employed: (1) Only Na, Ca, and Mn^{2+} were allowed at the X site; (2) Na and Ca were not allowed at any site other than X and (3) only Fe^{3+} and Al were allowed at the $M3a$ and $M3b$ sites. It should be noted that, without the last of these constraints, OccQP places some Mn^{3+} at the $M3a$ and $M3b$ sites; however, we think it is unlikely that significant Mn^{3+} is accommodated at these sites because Mn^{3+} typically generates Jahn-Teller distortion of octahedral coordinations and there is no evidence of such distortion around the $M3a$ and $M3b$ sites.

In the OccQP computations, different weighting schemes were applied to the compositional data for the Sapucaia and White Rock material. For Sapucaia, unit weights were used for chemistry, charge, valence, and

TABLE 7. SELECTED BOND DISTANCES (Å) AND ANGLES (°) FOR JAHNSITE-(NaMnMg) FROM SAPUCAIA

X–O1 (×2)	2.384(2)	$M2a$–O6 (×2)	2.0453(17)	$M3a$–OH (×2)	2.0007(16)
X–O7 (×2)	2.4867(18)	$M2a$–OW2 (×2)	2.105(2)	$M3a$–O7 (×2)	2.0103(17)
X–O5 (×2)	2.513(2)	$M2a$–OW3 (×2)	2.121(2)	$M3a$–O3 (×2)	2.0203(18)
X–O3 (×2)	2.866(2)	<$M2a$–O>	2.099	<$M3a$–O>	2.012
< X–O>	2.562				
		$M2b$–O2 (×2)	2.0255(19)	$M3b$–O8 (×2)	1.9843(17)
$M1$–O5 (×2)	2.0349(19)	$M2b$–OW4 (×2)	2.080(2)	$M3b$–OH (×2)	2.0106(16)
$M1$–O4 (×2)	2.1318(17)	$M2b$–OW1 (×2)	2.150(2)	$M3b$–O4 (×2)	2.0345(16)
$M1$–O1 (×2)	2.173(2)	<$M2b$–O>	2.097	<$M3b$–O>	2.015
< $M1$–O>	2.129				

		Hydrogen bonds					
P1–O2	1.4976(19)						
P1–O3	1.5164(18)	D–H⋯A	D–H	H⋯A		D⋯A	<D–H–A
P1–O1	1.552(2)	OH–H⋯OW2	0.78(2)	2.33(2)		3.095(3)	168(3)
P1–O4	1.5787(18)	OW1–H1a⋯O5	0.82(2)	1.98(2)		2.785(3)	166(3)
<P1–O>	1.536	OW1–H1b⋯OH	0.90(2)	2.24(2)		3.130(3)	170(3)
		OW2–H2a⋯OH	0.83(2)	2.27(3)		3.095(3)	173(3)
P2–O6	1.5113(19)	OW2–H2b⋯O1	0.86(2)	1.79(2)		2.648(3)	174(3)
P2–O8	1.5302(18)	OW3–H3a⋯OW1	0.77(2)	2.61(3)		3.133(3)	127(3)
P2–O7	1.5325(18)	OW3–H3b⋯O2	0.75(2)	2.12(2)		2.861(3)	169(4)
P2–O5	1.5527(18)	OW4–H4a⋯O6	0.75(2)	2.01(2)		2.751(3)	174(3)
<P2–O>	1.532	OW4–H4b⋯O8	0.76(2)	2.30(2)		3.048(3)	170(4)

average bond length. This allowed the composition to vary somewhat from the EPMA in order to optimize the fit with the structure refinement. For White Rock study, unit weights were used for charge, valence, and average bond length, but weights of 1000 were used for the EPMA data. The latter scheme allowed us to better allocate the cation content indicated by the EPMA empirical formula to structural sites and, most importantly, to apportion the Mn as Mn^{2+} and Mn^{3+}.

The results of the OccQP site population analyses for both Sapucaia and White Rock jahnsite-(NaMnMg) are provided in Table 6. These analyses clearly show

TABLE 8. BOND-VALENCE ANALYSIS FOR JAHNSITE-(NaMnMg) FROM SAPUCAIA
(VALUES ARE EXPRESSED IN VALENCE UNITS)

	X ×2↓	$M1$ ×2↓	$M2a$ ×2↓	$M2b$ ×2↓	$M3a$ ×2↓	$M3b$ ×2↓	P1	P2	Hydrogen bonds		Σ
									accepted	donated	
O1	0.23	0.34					1.20		0.26		2.03
O2				0.39			1.37		0.16		1.92
O3	0.07			0.48			1.31				1.86
O4		0.38				0.47	1.12				1.97
O5	0.17	0.48						1.20	0.19		2.04
O6			0.40					1.33	0.20		1.93
O7	0.18				0.49			1.26			1.93
O8						0.54		1.27	0.12		1.93
OH					0.51	0.50			0.11, 0.11	−0.11	1.12
OW1				0.30					0.11	−0.19, −0.11	0.11
OW2			0.35						0.11	−0.11, −0.26	0.09
OW3			0.34							−0.11, −0.16	0.07
OW4				0.35						−0.20, −0.12	0.03
Σ	1.30	2.40	2.18	2.08	2.96	3.02	5.00	5.06			

Bond strengths based upon cation site occupancies. Bond valence parameters are from Gagné & Hawthorne (2015). Hydrogen-bond strengths are based on O–O bond lengths from Ferraris & Ivaldi (1988).
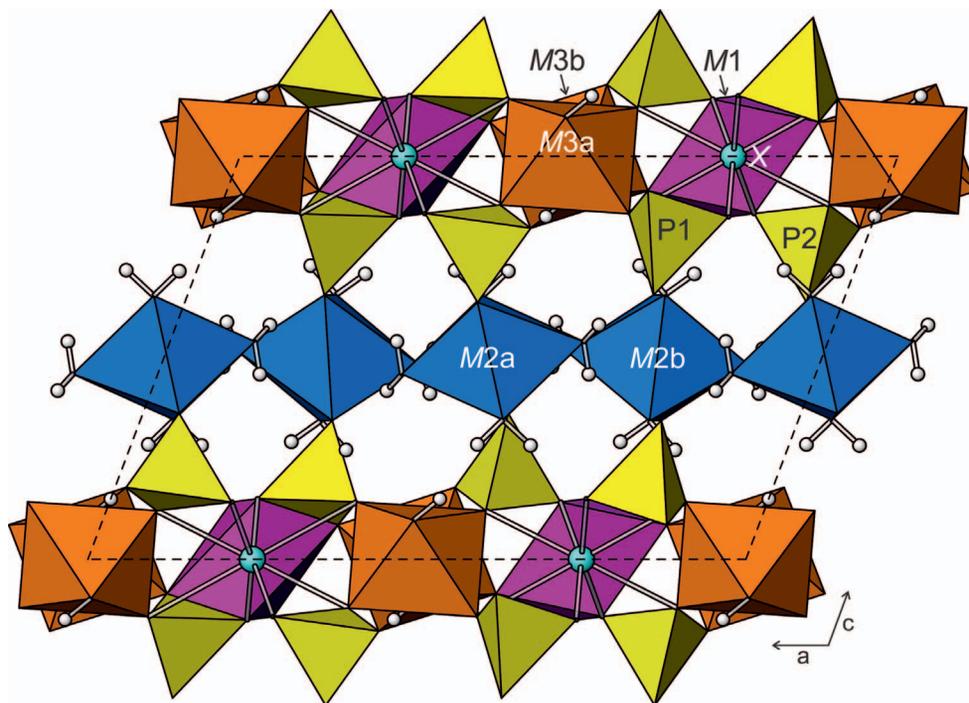
FIG. 5. The structure of jahnsite-(NaMnMg) viewed along [010]. X–O and O–H bonds are shown as sticks. Hydrogen bonds are not shown. The unit-cell outline is dashed.

that these jahnsites from both occurrences both conform to jahnsite-(NaMnMg). The OccQP analysis of White Rock material indicated that Mn should be apportioned as $Mn^{2+}_{0.752}Mn^{3+}_{0.248}$ and this was used for assigning MnO and Mn_2O_3 in the EPMA analyses (Table 2) and for the empirical formula. It is worth noting that even when Mn^{3+} was allowed at the $M3$ sites, the OccQP analysis of White Rock site populations was consistent with this material being jahnsite-(NaMnMg).

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