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Pumpellyite-(Al), a new mineral from Bertrix, Belgian Ardennes

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Abstract: Pumpellyite-(Al), ideally $Ca_2(Al,Fe^{2+},Mg)Al_2(SiO_4)(Si_2O_7)(OH,O)_2{\cdot}H_2O$, is a newly approved mineral species from Bertrix, Ardennes mountains, Belgium. It occurs as radiating fibrous aggregates reaching 5 mm in diameter, constituted by acicular crystals associated with calcite, K-feldspar and chlorite. Pumpellyite-(Al) is transparent to translucent and exhibits an emerald-green to white colour, sometimes with bluish tinges. The lustre is vitreous and the streak is colourless. The mineral is non-fluorescent, brittle, and shows a perfect {100} cleavage. The estimated Mohs hardness is 5½, and the calculated density is 3.24 g/cm^3. Pumpellyite-(Al) is biaxial positive, $\alpha = 1.678(2)$, $\beta = 1.680(2)$, $\gamma = 1.691(1)$ ($\lambda = 590$ nm), colourless in thin section, $2V = 46°$, $Y = b$, no dispersion. Electron-microprobe analyses gave SiO_2 37.52, Al_2O_3 25.63, MgO 1.99, FeO 4.97, MnO 0.11, CaO 23.21, BaO 0.01, Na_2O 0.03, K_2O 0.02, $H_2O_{calc.}$ 6.71, total 100.20 wt. %. The resulting empirical formula, calculated on the basis of 8 cations, is $(Ca_{1.99}Na_{0.01})_{\Sigma 2.00}(Al_{0.42}Fe^{2+}_{0.33}Mg_{0.24}Mn_{0.01})_{\Sigma 1.00}Al_{2.00}(SiO_4)(Si_2O_7)(OH)_{2.42} \cdot 0.58H_2O$. The simplified formula is $Ca_2AlAl_2(SiO_4)(Si_2O_7)(OH)_3$, which requires SiO_2 38.16, Al_2O_3 32.38, CaO 23.74, H_2O 5.72, Total 100.00 wt. %. The unit-cell parameters, refined from X-ray powder diffraction data, are: $a = 8.818(2)$, $b = 5.898(2)$, $c = 19.126(6)$ Å, $\beta = 97.26(3)°$, $V = 986.7(4)$ Å^3, space group $A2/m$. The eight strongest lines in the powder pattern [d-values(in Å)(I)(hkl)] are: 4.371(65)(200), 3.787(80)(202), 3.040(70)(204), 2.912(95)(300), 2.895(100)($30\bar{2}$), 2.731(40)($20\bar{6}$), 2.630(35)($31\bar{1}$), 2.191(45)($40\bar{2}$). Pumpellyite-(Al) belongs to the pumpellyite group, and corresponds to the Al-rich compositions where the M1 and M2 sites contain Al as predominant cation. The crystal structure of pumpellyite-(Al) has been refined by the Rietveld method, based on an X-ray powder diffraction pattern, to $R_{Bragg} = 7.09$ %. The infrared spectrum is similar to those of minerals of the pumpellyite group. The mineral species and name were approved by the Commission on New Minerals and Mineral Names, IMA (no. 2005-016).

Key-words: Pumpellyite-(Al), new mineral, crystal structure, infrared spectrum, Bertrix, Belgium.

Introduction

In the metamorphic area of Libramont-Bertrix, Belgian Ardennes, the occurrence of zeolites was first mentioned by Antun (1953) who described laumontite samples from the Cambrian Serpont Massif. More recently, the discovery of three new occurrences of this mineral around Bertrix initiated a detailed mineralogical study of laumontite from this area (Hatert, 1998), followed by the description of other zeolites, of prehnite, and of pumpellyite, associated with laumontite (Hatert & Theye, 2005).

In the Lochkovian schists and quartzites exploited in the Bertrix quarry, some fractures are covered by emerald-green to white radiating fibrous aggregates of acicular crystals. The aggregates, up to 5 mm in diameter, are associated with calcite, K-feldspar and chlorite. A preliminary examination by X-ray powder diffraction indicated that this mineral belongs to the pumpellyite group, and electron-microprobe analyses revealed the presence of aluminium in significant amounts (Hatert & Theye, 2005).

Occurrences of Al-rich pumpellyite were previously reported in literature, and the crystal structures of several Al-rich pumpellyite samples were published by Galli & Alberti (1969), Yoshiasa & Matsumoto (1985), Artioli & Geiger (1994), and Artioli *et al.* (1996). The name "pumpellyite-(Al)" was proposed by Passaglia & Gottardi (1973) for samples with Al-rich compositions, but the physical properties of the mineral and its crystal structure were not determined. The report of Passaglia & Gottardi (1973) with the nomenclature of the pumpellyite group was approved by the Commission on New Minerals and Mineral Names of the International Mineralogical Association (CNMMN-IMA). However, as no formal proposal has been submitted to the CNMMN, the status of pumpellyite-(Al) as a valid species was still controversial. The mineral does not appear in Dana's New Mineralogy (Gaines *et al.*, 1997), in the Handbook of Mineralogy (Anthony *et al.*, 1997), or in the Encyclopedia of Mineral Names (Blackburn & Dennen, 1997). Hey's Mineral Index (Clark, 1993) gives the name, but not in bold type, meaning that it is not considered as a species. The

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Strunz Mineralogical Tables (Strunz & Nickel, 2001), however, list pumpellyite-(Al) as a valid mineral.

The aim of this paper is to fill the gap in systematic mineralogy with a complete description of a sample of pumpellyite-(Al). Comprehensive data, namely physical, optical, infrared spectral, chemical, X-ray powder diffraction data, and a Rietveld structure refinement, are here presented for the same sample, which from now on has to be considered as the holotype. The mineral is named in accordance with the nomenclature of the pumpellyite group (Passaglia & Gottardi, 1973) and with the CNMMN-IMA rules. The mineral species and name were approved by the CNMMN-IMA (no. 2005-016), and the type material is stored in the collection of the Laboratory of Mineralogy, University of Liège, Belgium (no. 20327).

Geological setting

Many samples of pumpellyite-(Al) were collected between 1998 and 2003 in the quarry "Carrière de la Flèche", 3 km northwest of the Bertrix village, Belgian Ardennes. The mineral occurs in lately formed veins associated with calcite, K-feldspar and chlorite. The veins crosscut metamorphic quartzites and schists of Lochkovian sedimentation age, with a primary metamorphic assemblage comprising minerals such as magnetite, plagioclase, biotite, as well as rare hornblende and garnet. Low P-medium T conditions around 2 kbar / 400°C are estimated by Beugnies (1986). Data obtained by Theye & Fransolet (1993) on assemblages containing garnet, plagioclase, and hornblende indicate maximum P-T conditions up to 3–4 kbar / 500°C in the area of Libramont.

The formation of the late minerals, such as zeolites (laumontite, stilbite-Ca, chabazite-Ca, natrolite and/or tetranatrolite), prehnite, pumpellyite-(Al), chlorite, microcline, and calcite, is related to the retrograde, low-temperature alteration of the metasediments. The decomposition of biotite released Fe and Mg for the formation of pumpellyite-(Al) and chlorite, and K for the formation of microcline. The replacement of plagioclase by albite was the source of Ca for secondary minerals. Particularly, laumontite crystallised at a pressure of 2 +/- 1 kbar and between 200 and 250°C (Hatert & Theye, 2005). Stilbite-Ca appeared between 150 and 250°C, and the maximum stability ranges of prehnite and pumpellyite-(Al) are compatible with the stability field of associated laumontite (Hatert & Theye, 2005).

Physical properties

Pumpellyite-(Al) aggregates (Fig. 1), up to 5 mm in diameter, show an emerald-green to white colour, sometimes with distinct bluish tinges. The mineral is transparent to translucent, with a vitreous lustre and with a colourless streak. It is non-fluorescent, brittle, and shows a perfect {100} cleavage. The estimated Mohs hardness is 5½. The density could not be measured due to the fibrous habit of the mineral; the calculated density is 3.24 g/cm^3. Pumpellyite-(Al) is biaxial positive, with $\alpha = 1.678(2)$, $\beta = 1.680(2)$, and $\gamma = 1.691(1)$ ($\lambda = 590$ nm). The mineral is colourless in thin section, and the calculated $2V$ angle is 46°. Y is oriented along the b axis, and no dispersion has been observed.

Infrared spectroscopy

The infrared spectrum of pumpellyite-(Al) (Fig. 2) was recorded with a Nicolet NEXUS spectrometer, from 32 scans with a 1 cm^{-1} resolution, over the 400–4000 cm^{-1} region.

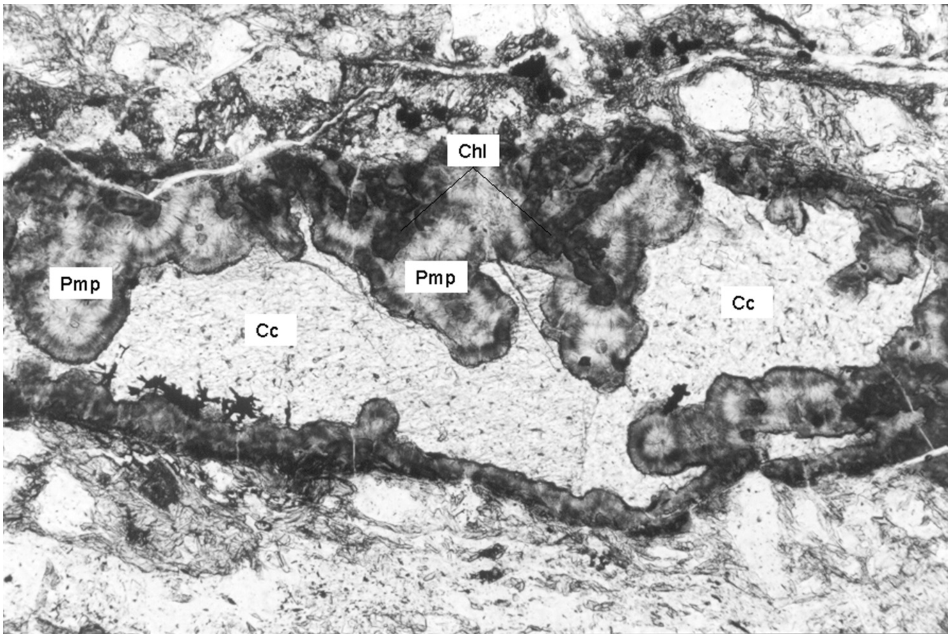

Fig. 1. Fibrous radiating aggregates of pumpellyite-(Al) (Pmp), associated with calcite (Cc) and chlorite (Chl) from Bertrix, Belgium. Transmitted light polarising microscope, 250 µm length.

The sample was prepared by intimately mixing 1 mg of sample with KBr in order to obtain a 150 mg homogeneous pellet which was subsequently dried for a few hours at 110°C. To prevent water contamination, the measurements were performed under a dry air purge.

The infrared spectrum is comparable to the vibrational spectra of other hydrous sorosilicates, as for example minerals of the epidote group (Liebscher, 2004) or västmanlandite-(Ce) (Holtstam *et al.*, 2005). The spectrum shows a complex group of broad bands at ca. 3542, 3499, 3407, 3127 and 3010 cm^{-1}, which can be assigned to OH stretching vibrations. The absence of an absorption band around 1630 cm^{-1}, which is typical for the bending vibrations of H_2O (Farmer, 1974), indicates that molecular water can occur only in very small amounts in pumpellyite-(Al). This last conclusion is in good agreement with the structural investigation of an Al-rich pumpellyite sample by Yoshiasa & Matsumoto (1985), and with the bond-valence calculations of Allmann & Donnay (1971), which did not show significant amounts of molecular water in the structure. In pumpellyite-(Al), the replacement of divalent cations by aluminium probably induces the replacement of molecular water by OH groups, according to the substitution mechanism $(Fe,Mg,Mn)^{2+} + H_2O \rightarrow Al^{3+} + OH^-$.

According to the correlation established by Libowitzky (1999), the wavenumbers of the observed OH stretching bands indicate the presence of OH…O hydrogen bonds, with distances 2.65 (3010 cm^{-1}), 2.68 (3127 cm^{-1}), 2.80 (3407 cm^{-1}), 2.89 (3499 cm^{-1}), and 2.98 Å (3542 cm^{-1}). These distances are in good agreement with those determined from the Rietveld refinement of the X-ray powder diffraction pattern of pumpellyite-(Al) (see below), thus confirming the consistency between our infrared and structural data.

At lower wavenumbers two very complex regions occur, corresponding to the antisymmetric stretching (ca. 1150–800 cm^{-1}) and bending vibrations (ca. 700–400 cm^{-1}) of the $[SiO_4]^{4-}$ and $[Si_2O_7]^{6-}$ groups (Farmer, 1974). The absorption band at 1129 cm^{-1} probably correspondens to the ν_{as}Si-O-Si vibrational mode of the $[Si_2O_7]^{6-}$ group, and according to Lazarev (1972), a correlation exists between the position of this band and the mean Si-O bond of the $[Si_2O_7]^{6-}$ group. The position of this band corresponds to a Si-O distance of 1.625 Å, close to the mean (Si1+Si2)-O bond length of 1.634 Å, obtained from the structural data (see below).

Chemical composition

Quantitative chemical analyses were performed with a Cameca SX-100 electron microprobe (Institut für Mineralogie und Kristallchemie, Universität Stuttgart, Germany) operated in the wavelength-dispersion mode, with an accelerating voltage of 15 kV, a beam current of 10 nA, and a beam diameter of 5 μm. The following standards were used: wollastonite (Si, Ca), corundum (Al), periclase (Mg), hematite (Fe), rhodonite (Mn), barite (Ba), albite (Na) and orthoclase (K).

The composition of pumpellyite-(Al) (Table 1) was calculated on the basis of 8 cations. The H_2O- and OH-contents

Table 1. Electron-microprobe analysis of pumpellyite-(Al).

Constituent	Wt. %	Range	Stand. Dev.	Composition (a.p.f.u.)
SiO_2	37.52	37.29–38.12	0.28	3.005
Al_2O_3	25.63	25.16–26.09	0.28	2.419
MgO	1.99	1.79–2.40	0.21	0.238
FeO^*	4.97	4.09–5.60	0.54	0.333
MnO	0.11	0.04–0.15	0.04	0.007
CaO	23.21	23.00–23.57	0.19	1.991
BaO	0.01	0.00–0.04	0.01	tr.
Na_2O	0.03	0.02–0.05	0.01	0.005
K_2O	0.02	0.00–0.04	0.01	0.002
H_2O^{**}	6.71			3.578
Total	100.20			

Analyst: T. Theye. Average of 7 analyses.

The composition was calculated on the basis of 8 cations per formula unit.

*: It is not necessary to introduce Fe^{3+} to maintain charge balance.

**: H_2O and OH^- groups were calculated to maintain charge balance.

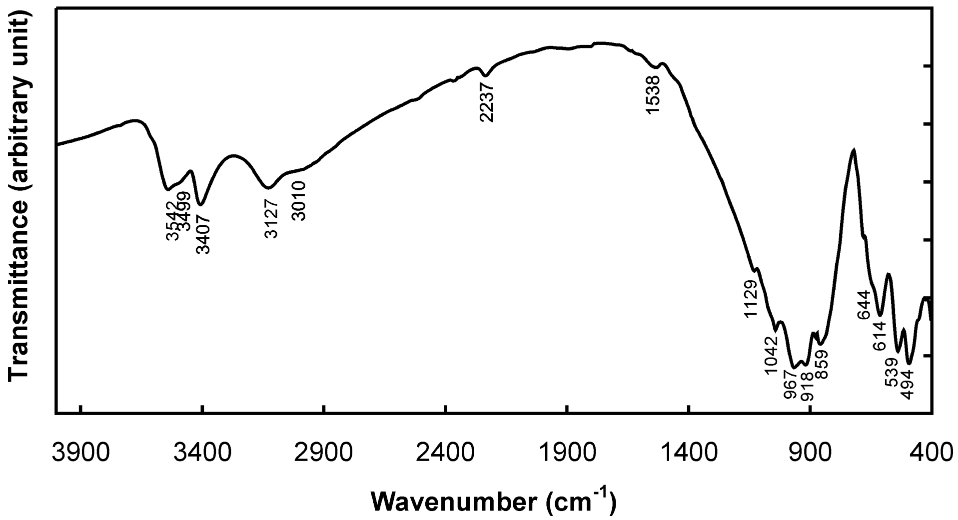

Fig. 2. Infrared spectrum of pumpellyite-(Al) from Bertrix, Belgium.

were calculated to maintain charge balance, according to the substitution mechanism $(Fe,Mg,Mn)^{2+} + H_2O \rightarrow Al^{3+} + OH^-$ (see above). It was not necessary to introduce Fe^{3+} to maintain charge balance. The empirical formula of pumpellyite-(Al) corresponds to $(Ca_{1.99}Na_{0.01})_{\Sigma 2.00}(Al_{0.42}Fe^{2+}_{0.33}Mg_{0.24}Mn_{0.01})_{\Sigma 1.00}Al_{2.00}(SiO_4)(Si_2O_7)(OH)_{2.42} \cdot 0.58H_2O$. The simplified formula is $Ca_2AlAl_2(SiO_4)(Si_2O_7)(OH)_3$, which requires SiO_2 38.16, Al_2O_3 32.38, CaO 23.74, H_2O 5.72, Total 100.00 wt. %.

X-ray powder diffraction

The X-ray powder diffraction pattern of pumpellyite-(Al), given in Table 2, was obtained with a PHILIPS PW-3710 diffractometer using Mn-filtered Fe*K*α radiation (λ = 1.9373 Å). The powder pattern is similar to those of other minerals of the pumpellyite group. On the basis of the *d*-spacings shown in Table 2, which were calibrated with an internal standard of $Pb(NO_3)_2$, the least-squares refinement

Table 2. X-ray powder diffraction pattern of pumpellyite-(Al) from Bertrix, Belgium.

I/I_0	$d_{obs.}$	$d_{calc.}$	h k l	I/I_0	$d_{obs.}$	dcalc.	h k l
35	8.735	8.748	1 0 0	15	2.157	2.157	0 2 6
30	4.739	4.743	0 0 4	15	2.112	2.114	2 2 4
35	4.661	4.657	1 1 1	25	2.089	2.089	4 0 $\bar{4}$
65	4.371	4.374	2 0 0	25	2.070	2.074	3 2 0
25	4.177	4.178	2 0 $\bar{2}$	15	2.004	2.004	2 2 $\bar{6}$
80	3.787	3.794	2 0 2	10	1.981	1.983	2 0 8
25	3.439	3.439	2 0 $\bar{4}$	20	1.913	1.914	1 3 $\bar{1}$
70	3.040	3.030	2 0 4	15	1.872	1.872	2 2 6
25	2.956	2.949	0 2 0	15	1.848	1.848	0 2 8
95	2.912	2.916	3 0 0	10	1.718	1.720	4 0 $\bar{8}$
100	2.895	2.892	3 0 $\bar{2}$	15	1.697	1.697	4 2 2
40	2.731	2.732	2 0 $\bar{6}$	10	1.672	1.672	5 1 $\bar{3}$
20	2.689	2.693	3 0 2	15	1.662	1.664	1 1 $\overline{11}$
35	2.630	2.630	3 1 $\bar{1}$	10	1.634	1.634	3 3 $\bar{1}$
30	2.505	2.505	0 2 4	20	1.593	1.592	1 1 11
30	2.445	2.445	1 1 $\bar{7}$	15	1.579	1.578	5 0 4
25	2.324	2.325	3 1 3	10	1.567	1.565	4 1 $\bar{9}$
20	2.280	2.276	3 1 $\bar{5}$	15	1.553	1.553	2 2 $\overline{10}$
15	2.238	2.239	2 2 $\bar{4}$	10	1.541	1.541	1 2 10
30	2.205	2.205	2 0 $\bar{8}$	15	1.512	1.512	5 2 $\bar{2}$
45	2.191	2.192	4 0 $\bar{2}$				

Table 3. Final fractional coordinates and displacement parameters for pumpellyite-(Al).

Site	x	y	z	U*
Ca1	0.2501(5)	½	0.3397(3)	4.1(1)
Ca2	0.1903(6)	½	0.1547(3)	4.1(1)
M1**	½	¼	¼	3.4(2)
M2**	0.2543(6)	0.2485(14)	0.4963(3)	2.5(1)
Si1	0.0556(9)	0	0.0934(4)	3.4(1)
Si2	0.1711(7)	0	0.2477(4)	3.4(1)
Si3	0.4627(9)	0	0.4042(4)	3.4(1)
O1	0.1415(9)	0.2230(15)	0.0703(5)	4.7(1)
O2	0.2793(9)	0.2265(11)	0.2452(5)	4.7(1)
O3	0.3701(9)	0.2286(12)	0.4171(5)	4.7(1)
O4	0.1243(11)	½	0.4408(8)	4.7(1)
O5	0.1256(14)	0	0.4590(8)	4.7(1)
O6	0.3662(12)	½	0.0478(8)	4.7(1)
O7	0.3706(14)	0	0.0315(8)	4.7(1)
O8	0.0389(13)	0	0.1776(4)	4.7(1)
O9	0.4830(13)	½	0.1755(5)	4.7(1)
O10	0.0658(13)	0	0.3129(6)	4.7(1)
O11	0.5097(14)	½	0.3188(7)	4.7(1)

* Five isotropic displacement parameter were refined, for Ca1-Ca2, M1, M2, Si1-Si2-Si3, and O1 to O11, respectively.

** Site occupancies (fixed): M1 = 75 % Al, 12.5 % Fe, 12.5 % Mg; M2 = 100 % Al.

program LCLSQ 8.4 (Burnham, 1991) has served to calculate the unit-cell parameters *a* = 8.818(2), *b* = 5.898(2), *c* = 19.126(6) Å, β = 97.26(3)°, *V* = 986.7(4) $Å^3$.

Structure refinement

The crystal structure of pumpellyite-(Al) was refined from an X-ray powder diffraction pattern measured with a Bruker D8-Advance diffractometer using CuK_α radiation (λ = 1.5418 Å). The powder of the mineral was checked for purity with a polarizing microscope, and then introduced in a glass capillary (3 cm long and 0.5 mm in diameter). Two data sets were collected, with 0.0156° step size, and 25 s (8 to 55° 2θ) or 50 s counting time (55 to 100° 2θ). The two scans were merged through the Bruker program EVA into a single one, which was then used for the Rietveld refinement, carried out with the GSAS/EXPGUI suite of programs (Larson & Von Dreele, 2000; Toby, 2001).

The Rietveld refinement was performed starting from the atomic coordinates of pumpellyite given by Galli & Alberti (1969). Some minor discrepancies in the fit between observed and calculated profiles were easily interpreted assuming a small (2.5 %) quartz admixture. The unit-cell parameters, obtained from the Rietveld refinement, are: *a* = 8.8006(2), *b* = 5.8991(1), *c* = 19.0804(4) Å, β = 97.401(2)°, *V* = 982.32(4) $Å^3$. These unit-cell parameters differ significantly from those refined with the LCLSQ program (see above), probably due to different alignments of both goniometers. However, due to the correction of the *d* values by comparison with an internal standard, the unit-cell parameters refined with the LCLSQ program are more reliable, even if they show larger standard deviations.

Whereas the M2 site is occupied by Al only, in keeping with the well-assessed crystal chemistry of pumpellyites, the site occupancy at the M1 site was refined, assuming full occupancy and refining Al (including the similarly light Mg) against Fe. The best agreement was obtained with 88 % Al (including Mg) + 12 % Fe. In the final refinement cycles, the occupancy was fixed as follows: 75 % Al, 12.5 % Mg, and 12.5 % Fe. These values resulted in the lowest R_{Bragg} and were in good agreement with the chemical data. The structural data thus confirmed that the M1 site contains Al as the dominant cation. After refinement, the *R* factor computed on 633 squared *F*'s was 0.0709, and the R_{wp} was 0.0205.

Discussion

Compatibility index

The compatibility index of pumpellyite-(Al) is calculated with the relationship proposed by Mandarino (1981). The calculation of K_P was performed with the calculated density of 3.24 g/cm^3. The compatibility index, $1-(K_P/K_C)$, is -0.013, which ranges in the category "superior" following Mandarino (1981).

Structural features

Final positional and displacement parameters for pumpellyite-(Al) are given in Table 3, whereas selected bond distances and the bond-valence sums are reported in Table 4. The basic features of the crystal structure of pumpellyite-(Al) are identical to those of the other members of the pum-

Table 4 . Selected interatomic distances (in Å), and bond-valence sums (in valence unit), for pumpellyite-(Al).

Ca1 – O3	2.337(8)	M1 – O2	1.937(8)	Si1 – O1	1.607(5)
Ca1 – O3	2.337(8)	M1 – O2	1.937(8)	Si1 – O1	1.607(5)
Ca1 – O4	2.345(15)	M1 – O11	1.969(8)	Si1 – O4	1.633(7)
Ca1 – O11	2.369(13)	M1 – O11	1.969(8)	Si1 – O8	1.634(7)
Ca1 – O2	2.457(9)	M1 – O9	2.041(7)	<Si1 – O>	1.620
Ca1 – O2	2.457(9)	M1 – O9	2.041(7)		
Ca1 – O8	2.522(12)	<M1 – O>	1.982	Si2 – O10	1.644(8)
<Ca1 – O>	2.403			Si2 – O2	1.645(5)
		M2 – O1	1.834(9)	Si2 – O2	1.645(5)
Ca2 – O1	2.296(10)	M2 – O7	1.876(10)	Si2 – O8	1.656(7)
Ca2 – O1	2.296(10)	M2 – O3	1.932(9)	<Si2 – O>	1.647
Ca2 – O10	2.412(11)	M2 – O5	1.932(11)		
Ca2 – O2	2.420(10)	M2 – O6	1.958(10)	Si3 – O3	1.611(5)
Ca2 – O2	2.420(10)	M2 – O4	2.078(10)	Si3 – O3	1.611(5)
Ca2 – O9	2.555(12)	<M2 – O>	1.935	Si3 – O9	1.651(8)
Ca2 – O6	2.714(15)			Si3 – O6	1.658(7)
<Ca2 – O>	2.445			<Si3 – O>	1.633
Ca1	2.19	O1	2.07	O7	1.09
Ca2	2.05	O2	1.99	O8	2.11
M1	2.58	O3	1.87	O9	1.86
M2	2.84	O4	1.97	O10	1.25
Si1	4.04	O5	0.94	O11	1.22
Si2	3.75	O6	1.92		
Si3	3.91				

Table 5. Comparison of bond distances and occupancy within octahedra in some pumpellyite-group minerals.

Sample	[1]	[2]	[3]	[4]	[5]	[6]	[7]	[8]	[9]	[10]
M1-O2 (x2)	1.937(8)	2.04(1)	2.063(3)	2.027(7)	2.038(8)	2.110(7)	2.018(4)	2.033(5)	2.05(1)	2.155(5)
M1-O9 (x2)	2.041(7)	2.03(1)	2.036(2)	1.99(1)	2.02(1)	2.022(9)	2.054(4)	2.028(4)	2.13(1)	2.103(7)
M1-O11 (x2)	1.969(8)	1.90(1)	1.925(2)	1.959(9)	1.898(8)	1.950(9)	1.936(4)	1.934(5)	2.05(1)	1.993(8)
<M1-O>	1.982	1.990	2.008	1.992	1.985	2.027	2.003	1.998	2.077	2.084
Site occupancy	$Al_{0.75}$ $Fe_{0.125}$ $Mg_{0.125}$	$Al_{0.50}$ $Mg_{0.35}$ $Fe_{0.15}$	$Al_{0.80}$ $Fe_{0.20}$	$Al_{0.51}$ $Mg_{0.36}$ $Fe_{0.13}$	$Al_{0.50}$ $Mg_{0.37}$ $Fe_{0.13}$	$Al_{0.43}$ $Mg_{0.32}$ $Fe_{0.25}$	$Al_{0.49}$ $Mn_{0.33}$ $Mg_{0.18}$	$Al_{0.44}$ $Mg_{0.29}$ $Mn_{0.27}$	$Fe_{0.69}$ $Al_{0.31}$	${Fe^{3+}}_{0.52}$ ${Fe^{2+}}_{0.48}$
M2-O1	1.834(9)	1.84(1)	1.878(2)	1.89(1)	1.90(1)	1.94(1)	1.946(5)	1.866(6)	2.06(1)	2.005(5)
M2-O3	1.932(9)	1.87(1)	1.896(2)	1.91(1)	1.99(1)	1.90(1)	1.914(5)	1.925(5)	2.07(1)	2.002(5)
M2-O4	2.078(10)	2.04(1)	2.026(2)	2.04(1)	2.04(1)	2.001(9)	2.022(5)	1.964(5)	2.09(1)	2.095(7)
M2-O5	1.932(11)	1.93(2)	1.888(2)	1.920(9)	1.916(9)	1.902(8)	1.928(5)	1.897(6)	2.05(2)	1.993(8)
M2-O6	1.958(10)	1.94(2)	1.937(2)	1.932(9)	1.92(1)	1.970(9)	2.058(5)	2.034(5)	2.00(1)	2.003(7)
M2-O7	1.876(10)	1.89(2)	1.882(2)	1.922(8)	1.934(8)	1.984(8)	1.929(5)	1.945(6)	2.02(2)	1.969(8)
<M2-O>	1.935	1.918	1.918	1.936	1.950	1.949	1.966	1.938	2.048	2.011
Site occupancy	Al	Al	Al	$Al_{0.97}$ $Fe_{0.03}$	$Al_{0.89}$ $Fe_{0.11}$	$Al_{0.71}$ $Fe_{0.29}$	$Al_{0.74}$ $Mn_{0.26}$	$Al_{0.90}$ $Mn_{0.10}$	Fe	${Fe^{3+}}_{0.94}$ $Al_{0.06}$

[1] pumpellyite-Al (this study)
[2] pumpellyite, Hicks Ranch, Sonora Co., California USA (Galli & Alberti, 1969)
[3] pumpellyite, Sanbagawa, Gumma Prefecture, Japan (Yoshiasa & Matsumoto, 1985)
[4] pumpellyite, Hicks Ranch, Sonora Co., California, USA (Artioli & Geiger, 1994)
[5] pumpellyite, Keweenawan, Michigan, USA (Artioli & Geiger, 1994)
[6] pumpellyite, Bulla, Italy (Artioli & Geiger, 1994)
[7] Mn-rich pumpellyite, Passo del Bracco, Eastern Ligurian Apennines, Italy (SN1) (Artioli *et al.*, 1996)
[8] Mn-rich pumpellyite, Passo del Bracco, Eastern Ligurian Apennines, Italy (SN5) (Artioli *et al.*, 1996)
[9] julgoldite, Bombay, India (Artioli *et al.*, 2003)
[10] julgoldite (Allmann & Donnay, 1973)

pellyite group: the structure is built up by columns of edge-sharing MO_6 ($M = Al^{3+}, Fe^{2+}, Mg^{2+}$) octahedra running along [010], which are linked together *via* ortho- and disilicate groups, and by Ca^{2+} cations located on 7-coordinated sites.

The bond-valence balance has been carried out using the parameters given by Brese & O'Keeffe (1991); those bonds involving M1 were weighted on the basis of the site occupancy given in Table 3 for the M1 site. The M1 site has the lower sum by comparison to the M2 site, and this is in good agreement with the partial $M^{3+} \Leftrightarrow M^{2+}$ substitution at the M1 site. The location of hydroxyl groups at the O5, O7, O10 and O11 sites (with the latter two oxygen atoms statistically playing a double donor/acceptor role) is also confirmed. The distances between oxygen atoms involved in the hydrogen bonding are as follows: 2.708 (O7…O7), 2.771 (O10…O5), 2.867 (O5…O5), and 2.915 Å (O11…O7). For a deeper insight on the hydrogen bond system in the pumpellyite structure see, e.g., Yoshiasa & Matsumoto (1985).

A comparison of M-O bond distances and occupancies of the octahedral sites in pumpellyite-group minerals is given in Table 5, and shows that the bond distances calculated for the sample from Bertrix are similar to those obtained for other Al-rich pumpellyite samples.

The structure type of pumpellyite is closely related to those of sursassite and ardennite, with which it forms a polytypic family (Pasero & Reinecke, 1991).

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