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CRYSTAL CHEMISTRY AND NOMENCLATURE OF PUMPELLYITES AND JULGOLDITES

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ABSTRACT

Eighteen descriptions of pumpellyites and julgoldite allow a review of the crystal chemistry of these minerals. This review is the basis of a new nomenclature of this mineral group: it is proposed to use only the two existing names, pumpellyite and julgoldite, with the addition of suffixes to properly specify the chemical composition. A complete correlation analysis between chemical composition and lattice constants was not performed because the present data are considered insufficient; total iron is correlative with cell volume, but does not have a definite structural meaning.

INTRODUCTION

The pumpellyite mineral series was the object of a thorough study by Coombs (1953); since then, additional pumpellyites have been described so that it is now possible to review the crystal chemistry of these minerals, and to propose a more detailed nomenclature that has been approved by the Commission on New Minerals and Mineral Names, I.M.A.

One of us (E.P.) is responsible for data collecting, screening and handling. The samples considered here are listed in Table 1. Analyses with the microprobe were not considered because they lack the ferrous iron determinations which are essential for classification purposes.

CRYSTAL CHEMISTRY

The crystal structure of pumpellyite was determined by Gottardi (1965) and refined by Galli & Alberti (1969). As Allmann & Donnay (1971) and Baur (1971) both exclude the presence of water molecules in pumpellyite, the chemical formula of this mineral can be written $W_8X_4Y_8Z_{12}O_{56-n}(OH)_n$ where W = Ca,K,Na; X = Mn,Fe'',Al; Y = Fe''',Al,Ti; and Z = Si. Small quantities of Mn and Fe'' can be shifted to the W-position, and the Z-position may be filled with Al, if necessary.

The W-site displays sevenfold coordination, the Z-site tetrahedral coordination; both X- and Y-sites show octahedral coordination, the Y-octahedra being a little smaller (average Y-O distance = 1.92Å) than the X-octahedra (1.99Å). Crystal-chemical laws suggest that the Y-sites are filled with the smallest ion of the group (Al). If the number of Al-atoms per unit cell is insufficient to fill the Y-sites, the second smallest ion (Fe''') has to be put therein; because of its high charge, Ti in minor quantities is also associated with the Y-positions. Galli & Alberti (1969), refining their Al-rich pumpellyite, found all iron in the X-site. Hence we propose the following rules to calculate the chemical formula of a mineral with the pumpellyite structure:

1. The unit cell content should be calculated on the basis of 56 oxygens.
2. Si-cations should be grouped together.
3. Seven-coordinated cations (Ca,K,Na) should be grouped together.
4. Octahedral cations (Mn, Fe'',Mg, Fe''', Al) should be grouped together; if their sum is

TABLE 1. SOURCES OF DATA

Sample number	Locality	Reference
1	Knockormal Farm, Lendalfoot, S. Ayrshire, Scotland	Bloxam (1958)
2	Toba, Sinsen-mura, Central Japan	Seki (1958)
3	Watiba, Higasititibu-mura, Central Japan	Seki (1958): chem. anal. Surdam (1969): cell dim.
4	Sibukawa, Central Japan	Seki (1961): chem. anal. Seki *et al.*(1960): powder data
5	Kanasaki, Kanto Mt., Japan	Seki (1961)
6	Kamuikotan, Mituisi Distr., Hokkaido, Japan	Seki (1961)
7	North Caucasus, USSR	Lupanova & Kudryavtsev (1963)
8	Noril'sk, USSR	Zolotukhin *et al.* (1965)
9	Mrovdag, Lesser Caucasus, USSR	Abdullaev & Azadaliev (1968)
10	Langban, Sweden	Allmann & Donnay (1973)
11	Calumet, Michigan, USA	Palache & Vassar (1925): chem. anal.; Coombs (1953): powder data
12	Mill Creek, Calif., USA	Irving *et al.* (1932)
13	Skaggs, California, USA	Irving *et al.* (1932)
14	Asahine, Tukikawa-mura, Saitama Pref., Japan	Tsuboi (1936)
15	Hicks Ranch, Calif., USA	Galli (1972a)
16	Tiso, Bolzano, Italy	Galli (1972b)
17	Bulla, Bolzano, Italy	Passaglia (1972)
18	Kotu-Bizan area, East. Sikoku, Japan	Iwasaki (1963)

TABLE 2. ATOMIC COEFFICIENTS IN THE CHEMICAL FORMULAE

Sample number	Position *W*						Position *X*						Position *Y*				Position *Z*				
	K	Na	Ca	Mn	Fe"	total	Mn	Fe"	Mg	Fe'''	Al	total	Fe'''	Al	Ti	total	Al	Si	total	O	OH
1		0.13	7.87			8.00	0.04	0.83	1.29	0.48	1.39	4.03		7.96	0.04	8.00	0.05	11.95	12.00	41.87	14.13
2	0.04	0.30	7.88			8.22	0.13	0.58	1.71	0.53	0.88	3.83		8.00		8.00		12.20	12.20	41.98	14.02
3	0.08	0.42	7.44			7.94	0.12	0.62	0.74	0.90	1.40	3.78		8.00		8.00		12.17	12.17	41.78	14.22
4	0.01	0.11	7.70			7.82	0.06	0.36	0.99	0.15	2.02	3.58		8.00		8.00		12.25	12.25	41.97	14.03
5	0.02	0.04	8.61			8.67		0.09	1.63	0.19	2.00	3.91		7.91	0.09	8.00		12.32	12.32	44.38	11.62
6		0.06	7.58	0.02	0.34	8.00		0.45	1.35	0.85	1.38	4.03		7.95	0.06	8.01		12.10	12.10	42.57	13.43
7	0.01	0.78	6.15	0.06	0.44	7.44		0.83	1.29	0.65	1.23	4.00		7.81	0.19	8.00		12.57	12.57	43.39	12.61
8		0.13	7.78	0.01	0.08	8.00		2.60	0.49	1.01		4.10	3.81	4.22	0.02	8.05		12.34	12.34	42.70	13.30
9	0.01	0.25	7.75			8.01	0.02	0.97	1.10	0.69	1.40	4.18		8.13	0.02	8.15		12.02	12.02	42.30	13.70
10*			8.00			8.00		1.92		2.08		4.00	7.52	0.48		8.00		12.00	12.00	42.08	13.92
11		0.12	7.94			8.06	0.03	0.56	1.52	1.24	0.76	4.11		8.08		8.08	0.06	11.94	12.00	42.54	13.46
12		0.28	7.76			8.04	0.05	0.77	0.86	0.26	1.78	3.72		7.95	0.05	8.00		12.13	12.13	41.87	14.13
13	0.03	0.28	7.27			7.58	0.28	0.86	0.69		2.08	3.91		7.90	0.10	8.00	0.12	11.88	12.00	40.69	15.31
14		0.36	7.75			8.11	0.03	0.79	1.27	0.42	1.56	4.07		8.04	0.03	8.07		12.03	12.03	42.38	13.62
15		0.20	7.59		0.21	8.00		0.55	1.41	0.18	1.95	4.09		8.00		8.00	0.84	11.16	12.00	41.31	14.69
16	0.03	0.15	7.56			7.74	0.04	0.77	1.28	1.13	0.47	3.69		7.97	0.03	8.00		11.90	11.90	39.89	16.11
17	0.02	0.28	7.34	0.01	0.23	7.88		0.54	1.53	1.93		4.00	0.84	7.14	0.02	8.00	0.16	11.84	12.00	41.35	14.65
18	0.10	0.11	7.73			7.94	0.02	0.52	1.02	0.87	1.49	3.92		7.94	0.06	8.00		12.00	12.00	42.09	13.91

* For sample 10, atomic coefficients calculated by Allmann & Donnay (1973) from structure refinement and two microprobe analyses; ratio Fe":Fe''' deduced from the value of Moore (1971) corrected for ilvaite impurities.

higher than 12, part can be shifted, without lowering this sum under 12, as follows: (a) if the sum of Si is less than 12, part of the Al can be added to Si to reach a total of 12 tetrahedral cations; (b) if the sum of seven-coordinated cations (Ca,K,Na) is less than 8, Mn″ and, if necessary, part of Fe″, can be added to reach a total of 8 seven-coordinated cations.

5. The 12 (or less) octahedral cations are then divided into the *X*-position of equipoint 4 and the *Y*-position of equipoint 8, as follows: (a) Al and Ti are inserted in the *Y*-position; if this insertion is insufficient to reach a total of eight cations, Fe‴ is added until the site is full; (b) Mn,Fe″,Mg are set in the *X*-position, together with Fe‴ and Al, if some remains free after their assignment to the *Y*-position.

After this distribution some imbalance may still remain: for example, Si may exceed 12 or (Ca,K,Na) may exceed 8; this imbalance is left as such because it is considered to be due to analytical errors. The same holds if (Mn,Fe″, Mg,Fe‴,Al) exceeds 12 after shifting part to the *Z*-position and *W*-position. If the octahedral cations are less than 12, the proposed calculation accumulates the whole deficit in the *X*-position.

Following these rules, the chemical formula of the minerals listed in Table 1 have been calculated and listed in Table 2. Table 3 shows the percentage of cations in *X* and *Y* in the same minerals. From inspection of Table 3, it may be stated:

In position *Y*, Al is always the predominant cation, except in mineral no. 10 (julgoldite), where Fe‴ is predominant.

In position *X*, the predominant cation may be: Al in no. 1,3,4,5,6,9,12,13,14,15,18; Fe‴ in no. 17,10; Mg in no. 2,7,11,16; Fe″ in no. 8.

NOMENCLATURE

The following nomenclature is proposed: minerals with the pumpellyite structure are named pumpellyite if Al is predominant in the *Y*-position, and julgoldite if Fe‴ is predominant in the *Y*-position. The minerals may be distinguished further by means of a suffix that denotes the cation which predominates in the *X*-position. Thus, for samples 1,3,4,5,6,9,12,13,14,15,18, the name pumpellyite-(Al) may be applied. Sample 17 is pumpellyite-(Fe‴). Pumpellyite-(Fe″) is the proper name for sample 8, whereas pumpellyite-(Mg) is the name we propose for samples 2,7,11,16. The new mineral found by Moore (1971) could be named precisely julgoldite-(Fe‴) (sample 10). New types of pumpellyite

TABLE 3. OCCUPANCIES (%) IN POSITIONS *X* AND *Y* *

Sample no.	Position *X*					Position *Y*		
	Mn	Fe^{2+}	Mg	Fe^{3+}	Al	Fe^{3+}	Al	Ti
1	1.0	20.6	32.0	11.9	**34.5**		**99.5**	0.5
2	3.4	15.1	**44.7**	13.8	23.0		**100.0**	
3	3.1	16.4	19.5	23.8	**37.0**		**100.0**	
4	1.6	10.0	27.6	54.1	**56.4**		**100.0**	
5		2.3	41.6	4.8	**51.1**		**98.9**	1.1
6		11.1	33.4	21.0	**34.2**		**99.3**	0.7
7		20.7	**32.3**	16.2	30.8		**97.6**	2.4
8		**63.4**	12.0	24.6		47.3	**52.5**	0.2
9	0.5	23.2	26.3	16.5	**33.5**		**99.8**	0.2
10		48.0		**52.0**		**94.0**	6.0	
11	0.7	13.6	**37.0**	30.2	18.5		**100.0**	
12	1.3	20.7	23.1	7.0	**47.8**		**99.4**	0.6
13	7.2	22.0	17.6		**53.2**		**98.7**	1.3
14	0.7	19.4	31.2	10.3	**38.3**		**99.6**	0.4
15		13.4	34.5	4.4	**48.7**		**100.0**	
16	1.1	20.8	**34.7**	30.6	12.7		**99.6**	0.4
17		13.5	38.2	**48.3**		10.5	**89.3**	0.2
18	0.5	13.3	26.0	22.2	**38.0**		**99.2**	0.8

* The highest percentage in each position is underlined.

For Fe^{3+} in sample 4 read 4.1.

and julgoldite, not yet known, could be easily inserted in such a scheme of nomenclature.

It is important to notice that this nomenclature has the same basis as the scheme proposed by Moore (1971), *i.e.* cation occupancies in X- and Y-sites (see Table 4). However, Moore's scheme requires that a pumpellyite have more than 50% of an ion in each position to deserve a name. As in the majority of these minerals there is no ion with an occupancy factor higher than 50%, there is no name for them in Moore's scheme. In other words, Moore's proposal simply cannot be applied. In Moore's scheme one could not call an incompletely characterized member of the group simply "pumpellyite", because this would have a well-defined meaning (more than 50% of Mg in X, more than 50% of Al in Y). In our proposal, on the contrary, one can always use the name pumpellyite without a suffix if the occupancies in X are not known, or if one does not prefer our system of suffixes.

Moore's names and our names differ in several aspects, but mainly because he uses prefixes, whereas we propose suffixes which have well-known advantages. In particular all these minerals remain united in every alphabetical list.

Apart from the drawback of every such scheme of nomenclature for solid solution series, *i.e.* boundaries are defined where no boundaries exist, our nomenclature has two drawbacks of its own:

1. A mineral rich in Fe''' may receive a name which does not emphasize this aspect of its composition because with Fe''' being distributed both in X- and Y-sites, it may not be the most abundant cation either in X or in Y. This is the case of mineral no. 8 which is a pumpellyite-(Fe'') although it has, on the whole, $Fe''' > Al$ and $Fe''' > Fe''$. In Moore's nomenclature the mineral would be called "ferropumpellyite". This, in our point of view, is not a real drawback, but simply a consequence of a choice: emphasizing the ions which predominate in sets of equipoints more than the ions which predominate in the crystal as a whole. The mineral could, however, be termed "ferrian pumpellyite-(Fe'')".

TABLE 4. COMPARISON OF PROPOSED NOMENCLATURE WITH THAT PROPOSED BY MOORE (1971)*

Name suggested in this paper	X	Y	Name suggested by Moore (1971)
Pumpellyite-(Mg)	Mg	Al	Pumpellyite
Pumpellyite-(Fe")	Fe"	Al	Ferropumpellyite
Pumpellyite-(Fe''')	Fe'''	Al	Oxyferropumpellyite
Julgoldite-(Mg)	Mg	Fe'''	Ferripumpellyite
Julgoldite-(Fe")	Fe"	Fe'''	Julgoldite
Julgoldite-(Fe''')	Fe'''	Fe'''	Oxyjulgoldite

* For the nomenclature proposed in this paper, the listed cations must be the most abundant; for Moore's (1971) names the occupancy must be greater than 50%.

2. It is possible to find a pumpellyite-(Mg) with less Mg in X than a pumpellyite-(Al); this happens in sample no. 7 [pumpellyite-(Mg) with 32% of Mg in X] and sample no. 5 [pumpellyite-(Al) with 41% of Mg in X, but with 52% of Al in X]. This is a real drawback, but we still do not feel there is a better alternative. On the other hand, for minerals whose most abundant cation in X has a very low occupancy percentage, the suffix could be omitted; we do not suggest any minimum value to maintain the suffix.

UNIT CELL DIMENSIONS

Unit cell parameters are available for samples listed in Table 5, which are only part of those grouped in Table 1. Wherever possible, the parameters have been newly-obtained by least squares treatment of the published powder data using the indexing of Galli (1972a), who took into account diffraction intensities as measured in single crystals. Differences between Galli's (1972a) and Coombs' (1953) indexing are negligible, the exception probably being due to a printing error: the 2.64Å line is indexed at (311) by Coombs, and as $(31\bar{1})$ by Galli (1972a) and by Seki *et al.* (1960).

A few detailed comments on the values in Table 5 are warranted. For sample 2, Seki (1958) obtained $a = 8.83$, $b = 5.91$, $c = 19.14$Å, $\beta = 97°36'$ from his powder data. These values are slightly different from our calculated results as given in Table 5. For sample, Surdam's (1969) original values, as obtained from unpublished powder data, have been accepted. The parameters for sample 8 differ substantially from those reported by Zolotukhin *et al.* (1966), who obtained $a = 8.49$, $b = 5.99$, $c = 19.40$Å, $\beta = 100.4°$. However Zolotukhin *et al.* (1966) incorrectly indexed the $(31\bar{1})$ line, failed to index the 2.11Å line as $(40\bar{4})$, used the weak (300) line, and indexed as (204) a line at 3.34Å that is probably due to quartz. For sample 10, the parameters of

TABLE 5. LATTICE CONSTANTS OF THE PUMPELLYITES (error in brackets)

Sample no.	a(Å)	b(Å)	c(Å)	β	V(Å^3)
3	8.81	5.89	19.12	97°24'	983.89
2	8.831(4)	5.894(5)	19.10(1)	97°32'(3')	985.57
15	8.8204(3)	5.9038(3)	19.118(1)	97°24'42"(13")	987.22
18	8.814(7)	5.920(6)	19.09(2)	97°33'(6')	987.56
16	8.816(1)	5.918(1)	19.118(2)	97°25'(1')	989.10
11	8.826(3)	5.919(4)	19.142(9)	97°27'(2')	991.56
4	8.851(8)	5.911(8)	19.13(2)	97°17'(5')	992.98
17	8.825(2)	5.945(3)	19.131(9)	97°27'(2')	995.23
8	8.89(2)	6.03(3)	19.19(4)	97°49'(12')	1020.51
10	8.922(4)	6.081(3)	19.432(9)	97°36'(4')	1045.02

Allmann & Donnay (1973) are reported. For sample 11, our parameters deduced from Coombs' (1953) powder data are very similar to those obtained by Coombs from single crystal photographs on the same material (with some refinement of b from powder data) : $a = 8.81$, $b = 5.94$, $c = 19.14$Å, $\beta = 97.6°$.

Inspection of the data in Table 4 shows that 8 of the 10 samples have similar parameters, and 2 have notably larger values. This fact, and the restricted number of samples for which both chemical analyses and unit cell data are available, discourage a thorough correlation analysis. It is apparent, however that the variation of a is smaller than the variations of b and c ; all these lengths are positively correlated. The variation of β is small. There is positive correlation of total iron with cell volume (see Fig. 1), as already stated by Surdam (1969). As the structural meaning of total iron is not certain, we have plotted (Fig. 2) the quantity of trivalent iron in position Y against the cell volume, obtaining again a good correlation. If we extract from Table 4 the 7 samples with no Fe$'''$ in Y, and plot the quantity of Fe$''$ in X against cell volume, there is not even the slightest indication of a correlation. We believe that the Fe$'''$ content in Y is the main factor influencing the cell dimensions. More data are required to clarify the problem.

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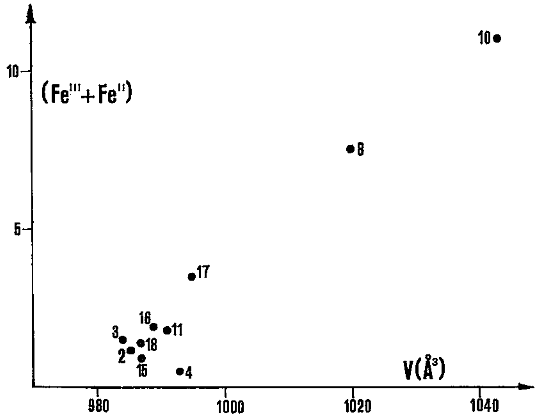

FIG. 1. Plot of total iron versus cell volume.

REFERENCES

ABDULLAEV, R.N. & AZADALIEV, G.A. (1968) : A find of pumpellyite in the Lesser Caucasus. *Zap. Vses. Min. Obshch.* **97,** 352-357.

ALLMANN, R. & DONNAY, G. (1971) : Structural relations between pumpellyite and ardennite. *Acta Cryst.* **B27,** 1871-1875.

——— & ——— (1973) : The crystal structure of julgoldite. (in press).

BAUR, W.H. (1971) : The prediction of bond length variations in silicon-oxygen bonds. *Amer. Mineral.* **56,** 1573-1599.

BLOXAM, T.W. (1958) : Pumpellyite from south Ayrshire. *Mineral. Mag.* **31,** 811-813.

COOMBS, D.S. (1953) : The pumpellyite mineral series. *Mineral. Mag.* **30,** 113-135.

GALLI, E. (1972a) : Nuovi dati sulla pumpellyite di Hicks Ranch (California). *Atti Soc. Tosc. Sci. Nat., Mem.* **[A]79,** 29-35.

——— (1972b) : La pumpellyite di Tiso-Theis (Bolzano). *Atti. Soc. Tosc. Sci. Nat., Mem.* **[A]79,** 23-28.

———, ALBERTI, A. (1969) : On the crystal structure of pumpellyite. *Acta Cryst.* **B25,** 2276-2281.

GOTTARDI, G. (1965) : Die Kristallstruktur von Pumpellyit. *Tschermaks Min. Petr. Mitt.* [3] **10,** 115-119.

IRVING, J., VONSEN, M. & GONYER, F.A. (1932) : Pumpellyite from California. *Amer. Mineral.* **17,** 338-342.

IWASAKI, M. (1963) : Metamorphic rocks of the Kotu-Bizan area, Eastern Sikoku. *J. Fac. Sci. Tokyo Univ.*, Sec. II, **15,** 1-90.

LUPANOVA, I.P. & KUDRYAVTSEV, V.T. (1963) : On the formula of pumpellyite. *Dokl. Acad. Sci. U.S.S.R., Earth Sci. Sec.* **141,** 1303-1306.

MOORE, P.B. (1971) : Julgoldite, the Fe^{+2}—Fe^{+3} dominant pumpellyite. *Lithos* **4,** 93-99.

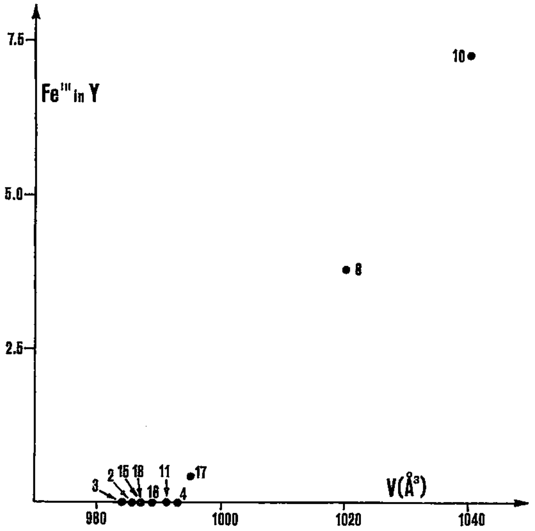

FIG. 2. Plot of trivalent iron in position Y versus cell volume.

Palache, C. & Vassar, H.E. (1925) : Some minerals of the Keweenawan copper deposits: pumpellyite, a new mineral; sericite; saponite. *Amer. Mineral.* **10,** 412-418.

Passaglia, E. (1972) : Pumpellyite fortemente ferrifera rinvenuta a Bulla (Bolzano). *Period Mineral.* **41,** 273-280.

Seki, Y. (1958) : Glaucophanitic regional metamorphism in the Kanto Mountains, central Japan. *Jap. Journ. Geol. Geogr.* **29,** 233-258.

———— (1961) : Pumpellyite in low-grade metamorphism. *J. Petrol.* **2,** 407-423.

———— Aiba, M. & Kato, C. (1960) : Jadeite and associated minerals of metagabbroic rocks in the Sibukawa district, central Japan. *Amer. Mineral.* **45,** 668-679.

Surdam, R.C. (1969) : Electron microprobe study of prehnite and pumpellyite from the Karmutsen Group, Vancouver Island, British Columbia. *Amer. Mineral.* **54,** 256-266.

Tsuboi, S. (1936) : Petrological notes (11). Pumpellyite from Asahine, Tukikawa-mura, Titibu-gori, Saitama Prefecture. *Jap. J. Geol. Geogr.* **13,** 333-337.

Zolotukhin, V.V., Vasil'yev, Yu. R. & Zyuzin, N.I. (1965) : Iron rich pumpellyite from the Noril'sk district and a new diagram for pumpellyites. *Dokl. Akad. Nauk U.S.S.R., Earth Sci.* **165,** 136-139.

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