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Wilancookite, (Ba,K,Na)₈(Ba,Li,□)₆Be₂₄P₂₄O₉₆·32H₂O, a new beryllophosphate with a zeolite framework

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Abstract: Wilancookite, ideally (Ba,K,Na)₈(Ba,Li, \square)₆Be₂₄P₂₄O₉₆·32H₂O, is a new mineral species from the Lavra Ponte do Piauí complex granitic pegmatite, Minas Gerais, Brazil. It occurs as tiny dodecahedral {110} crystals, deposited on moraesite fibres. Associated primary minerals are albite, montebrasite, Li-bearing micas, cassiterite, elbaite and quartz, while the secondary phosphate association contains fluorapatite, childrenite, eosphorite, zanazziite, greifenstenite, guimarãesite, ushkovite, saléeite and moraesite. The mineral is transparent and colourless, with a vitreous lustre; it is non-fluorescent, brittle, and its streak is white. The estimated Mohs hardness is 4–5, and the calculated density is 3.05 g/cm³. Wilancookite is isotropic, colourless, non-pleochroic, with *n* = 1.560(2) (measured under λ = 590 nm). Electron- and ion-microprobe analyses give (in wt%): P₂O₅ 36.19, SiO₂ 0.04, Al₂O₃ 0.41, BaO 34.65, Na₂O 0.09, K₂O 0.32, BeO 12.86, Li₂O 0.50, and H₂O_{calc} 12.31, total 97.37 wt%. The resulting empirical formula, calculated on the basis of 96 anhydrous oxygen atoms, is (Ba_{7.54}K_{0.32}Na_{0.14})_{\$\Structure 8.00}(Ba_{3.04}Li_{1.57} $\square_{1.39}$)_{\$\Structure 6.00}(Be_{24.08}(P_{23.88}Al_{0.38}Si_{0.03})_{\$\Structure 24.29} O₉₆·32H₂O. The single-crystal unit-cell parameters are *a* = 13.5398(2) Å and *V* = 2482.21(7) Å³, space group *I*23. The eight strongest lines in the powder X-ray diffraction pattern [*d*(in Å)(*I*)(*hkl*)] are: 6.90(60)(2 0 0), 5.54(80)(2 1 1), 3.630(60)(3 2 1, 3 1 2), 3.212(70) (3 3 0, 4 1 1), 3.043(100)(4 2 0, 4 0 2), 2.885(70)(3 3 2), 2.774(80)(4 2 2), and 2.398(60)(4 4 0). The crystal structure of wilancookite has been refined, based on single-crystal X-ray diffraction data, to *R*₁=4.58%; the beryllophosphate framework is similar to that occurring in pahasapaite, and is based on zeolite-RHO cages. The mineral species and name were approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogica

Key-words: wilancookite; new mineral; beryllophosphate; zeolite framework; crystal structure; pegmatite; Minas Gerais; Brazil.

1. Introduction

In Brazil occurs one of the most important pegmatite provinces in the world, the Eastern Brazilian Pegmatite Province (EBPP). This province is located at the East side of the Saõ Francisco craton, mainly in the state of Minas Gerais, but it encompasses also the states of Bahia, Espírito Santo and Rio de Janeiro (de Paiva, 1946; Putzer, 1976; Correia Nevez *et al.*, 1986). Pegmatites from this area are famous for their first-quality gems, but also for mineral systematics since 48 valid mineral species were first described in Minas Gerais (Atencio, 2000, 2008, 2015).

Wilancookite was discovered by Luiz Menezes in 2009, in the Lavra Ponte do Piauí complex granitic pegmatite. The mineral forms colourless tiny dodecahedral crystals, deposited on moraesite fibres. A preliminary examination by energy-dispersive spectrometry showed only Ba and P as major elements; X-ray single-crystal structure determination showed that the mineral was cubic (a = 13.5398(2) Å, space group *I*23), with a beryllophosphate structure topologically identical to that of zeolite-RHO (Nenoff *et al.*, 1996). The presence of Be was then confirmed by SIMS measurements, thus validating the new species.

Wilancookite, ideally $(Ba,K,Na)_8(Ba,Li,\square)_6Be_{24}P_{24}$ O₉₆·32H₂O, was accepted by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (CNMNC-IMA), under number IMA2015-034. The mineral is named to honour William R. Cook Jr. (1927–2006) and his wife Anne, who accepted to give their name to the mineral. Bill and Anne

number 20394), and in the collections of the Natural History Museum of Luxembourg (cotype used for chemical analyses: catalogue number 2011-33).

2. Occurrence and geological setting

Wilancookite occurs in the Lavra Ponte do Piauí complex granitic pegmatite, Itinga, Jequitinhonha, Minas Gerais, Brazil ($16^{\circ}43'33''$ S, $41^{\circ}53'55''$ W). The pegmatite is located in the Araçuaí pegmatite district, one of the subdivisions of the Eastern Brazilian Pegmatite province (Pedrosa-Soares *et al.*, 2011). The pegmatite has been mined for gemstones and samples for the collectors market. It is heterogeneous with well-developed mineralogical and textural zonation (Cassedanne & Philippo, 2015).

The pegmatite is hosted by biotite schist of the Neoproterozoic Salinas Group. The contact is not well exposed and did not allow to determine the orientation of the pegmatite body. A discontinuous quartz core is surrounded by small miarolitic cavities. The primary mineral association is represented by quartz, muscovite, microcline, schorl, and almandine–spessartine (Cassedanne & Philippo, 2015).

Wilancookite is a secondary mineral occurring in phosphate nodules adjacent to the quartz core of the pegmatite. Primary associated minerals are albite, montebrasite, Li-bearing micas, cassiterite, elbaite, and quartz. The secondary phosphate association contains fluorapatite, childrenite, eosphorite, zanazziite, greifenstenite, guimarãesite (Chukanov *et al.*, 2008), ushkovite, saléeite, and moraesite.

The primary phosphate occurring in this pegmatite is montebrasite. Beryllium-rich secondary phosphates formed during late stages, by reaction between montebrasite and beryl. This process produced several species, like beryllonite, greifenstenite, guimarãesite, moraesite, and zanazzite. Wilancookite crystallized in the very late conditions, since the crystals are deposited on moraesite fibres.

3. Physical properties

Wilancookite forms tiny dodecahedral {110} crystals, deposited on moraesite fibres (Fig. 1). The crystals are transparent, colourless, and reach a diameter of 100 μ m. The lustre is vitreous, the streak is white, and the mineral is non-fluorescent under either long or short-wavelength ultraviolet light. No cleavage has been observed, but the mineral is brittle with an irregular fracture. Mohs hardness is 4–5, by analogy with related pahasapaite (see below). The density could not be measured due to small grain size; the calculated density if 3.05 g/cm³. Wilancookite is isotropic, colourless, non-pleochroic, with n = 1.560(2) (measured under $\lambda = 590$ nm).

4. Chemical composition

Quantitative chemical analyses (Table 1) were performed on isolated crystals with a Cameca SX-50 electron microprobe (Ruhr-Universität Bochum, Germany) oper-

Fig. 1. Dodecahedral crystals of wilancookite, deposited on moraesite fibres. Lavra Ponte do Piauí pegmatite, Minas Gerais, Brazil. (a) Micro-photograph showing the clear colourless crystals; (b) scanning electron microscope image (secondary electrons mode) showing the dodecahedral morphology. (Online version in colour.)

endowed the mineralogy chair at the Cleveland Museum of Natural History; they were founding members of the Mineralogical Society of Cleveland and also of the Micromineral Society of the Cleveland Museum of Natural History. Bill was a mineralogist and crystallographer (BA from Oberlin, MA from Columbia, PhD from Case Western Reserve) (Clifford, 1997). The cotypes are deposited in the collections of the Laboratory of Mineralogy, University of Liège (cotype used for optics, crystal structure and Gandolfi measurements: catalogue



ating in the wavelength-dispersion mode, with an accelerating voltage of 15 kV, a beam current of 10 nA, and a beam diameter of $10 \mu\text{m}$. The following standards were used: AlPO₄ (P), andradite (Si), spessartine (Al), Baglass (Ba), jadeite (Na), and K-glass (K).

The Be and Li contents were determined with a Cameca IMS 4f ion microprobe installed at CNR-IGG, Pavia (Italy). We used a 12.5-kV accelerated ${}^{16}O^{-}$ primary-ion beam with a current intensity of 0.7 nA, corresponding to a beam diameter $<5 \,\mu$ m. The mount was polished, washed in an ultrasonic tank with ethanol, and Pt coated (400 Å thickness) before analysis. Secondary-ion signals of the isotopes ¹H⁺, ⁶Li⁺, ⁹Be⁺ and ³¹P⁺ were detected at the electron multiplier. The sample mount, together with the standard mount, was left to degas in the ion-probe sample chamber for a week before analysis under a 2×10^{-9} Torr vacuum. All measurements were done using secondary filtered ions in the range $\sim 75-125 \text{ eV}$ (Ottolini *et al.*, 1993, 2002; Hatert et al., 2011) under 25-µm imaged field and the 2[^] field aperture (750 µm diameter). Standard used for Li was triphylite from the Buranga pegmatite, Rwanda (Hatert et al., 2011); for Be we selected a sample of natural beryllonite which was previously analyzed by wet colorimetry and atomic absorption spectrophotometry $(BeO = 19.70 \text{ wt\%}; P_2O_5 = 55.90 \text{ wt\%}).$

The calibration factor for Li in the standard was obtained through the calculation of the experimental Li ion yield having chosen P as the internal reference element for the matrix. We thus derived the ion yield IY (Li/P), defined as $(Li^+/P^+)/((Li(at)/P(at)))$ where Li^+ and P^+ are the current intensities detected at the electron multiplier and (at) represents the elemental atomic concentration. It was done similarly for the IY(Be/P) from beryllonite. The two IYs were then used in wilancookite to calculate Li and Be concentrations reported in Table 1. The presence of H, through the ${}^{1}\text{H}^{+}$ signal, was confirmed by SIMS analysis but H₂O was not quantified due to the lack of proper calibration standard. The H₂O content of the formula was calculated according to the structural data. CO₂ was not determined but is considered absent according to the structural data.

The empirical formula of wilancookite, based on 96 anhydrous oxygen atoms per formula unit (*apfu*), is: $(Ba_{7.54}K_{0.32}Na_{0.14})_{\Sigma 8.00}(Ba_{3.04}Li_{1.57}\square_{1.39})_{\Sigma 6.00}Be_{24.08}$ (P_{23.88}Al_{0.38}Si_{0.03})_{\S24.29}O₉₆·32H₂O. The simplified formula is Ba₈(Ba₃Li₂])Be₂₄P₂₄O₉₆·32H₂O, which requires P₂O₅ 37.06, BeO 13.06, BaO 36.69, Li₂O 0.65, H₂O 12.54, total 100.00 wt%.

5. Raman spectroscopy

The Raman spectrum of wilancookite (Fig. 2) was collected from a randomly oriented crystal at 100% power, on a Thermo Almega Micro-Raman System, using a solid-state laser with a frequency of 532 nm and a thermoelectric cooled CCD detector. The laser was partially polarized with 4 cm^{-1} resolution and a spot size of 1 µm. The spectrum (Fig. 2) is characterized by peaks at

Table 1. Chemical analysis of wilancookite.

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Oxide	Mean (wt%)	Range	St. dev.	Cations pfu**
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	P_2O_5	36.19	33.39-37.29	1.18	23.88
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	SiO ₂	0.04	0.01 - 0.07	0.02	0.03
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Al ₂ Õ ₃	0.41	0.27-0.61	0.10	0.38
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	BaO	34.65	34.07-35.01	0.34	10.58
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Na ₂ O	0.09	0.06-0.13	0.03	0.14
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	K ₂ O	0.32	0.26-0.43	0.06	0.32
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	BeO	12.86	_	0.09	24.08
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Li ₂ O	0.50	_	0.01	1.57
Total 97.37 93.86–98.59 1.41	H_2O^*	12.31	_	_	64.00
	Total	97.37	93.86–98.59	1.41	

* Calculated according to the structural data.

** On the basis of 96 anhydrous oxygen atoms.

Ca and Sr are below detection limits.

430 (Be–O), 580 (ν_4 PO₄), 1000 (ν_1 PO₄), 1050 (ν_3 PO₄), 1600 (ν_2 H₂O), 3430 and 3680 (ν_3 H₂O) cm⁻¹. Band assignments were established according to the Raman data recently published for strontiohurlbutite, SrBe₂(PO₄)₂ (Dal Bo *et al.*, 2014; Rao *et al.*, 2014).

6. X-ray structure determination

The powder X-ray diffraction pattern of wilancookite, given in Table 2, was obtained with a Gandolfi camera (diameter 114.6 mm, exposure time 125 h) mounted on a PHILIPS PW-1730/10 X-ray generator using Ni-filtered CuK α radiation (λ =1.5418 Å). On the basis of the *d*-spacings shown in Table 2, and using the indexation obtained from the structural data, the least-squares refinement program LCLSQ 8.4 (Burnham, 1991) has served to calculate the unit-cell parameters of wilancookite: *a*=13.579(9) Å, and *V*=2504(5) Å³. The intensities, observed on the Gandolfi film, are in fairly good agreement with those calculated from the structural data (Table 2).

Single-crystal X-ray studies were carried out on an Rigaku Xcalibur 4-circle diffractometer (MoKα radiation, $\lambda = 0.71073$ Å), equipped with an EOS detector. A single crystal of wilancookite measuring $0.089 \text{ mm} \times 0.070 \text{ mm}$ \times 0.065 mm was mounted on a fibre lass; 49 frames with a spatial resolution of 1° were collected by the ϕ/ω scan technique, with a counting time of 700 s/frame, in the range $4.28^{\circ} < 2\theta < 57.14^{\circ}$. A total of 1292 reflections were extracted from these frames, corresponding to 805 unique reflections. The unit-cell parameters refined from these reflections, a = 13.5398(2) Å and V = 2482.21(7) Å³, are in good agreement with those refined from the X-ray powder data (see above). Data were corrected for Lorentz, polarization and absorption effects, the latter with an empirical method using the SCALE3 ABSPACK scaling algorithm included in the CrysAlisRED package (Agilent Technologies, 2012).

The crystal structure of wilancookite (Fig. 3) was refined in space group *I*23. Scattering curves for neutral atoms, together with anomalous dispersion corrections,



Fig. 2. The Raman spectrum of wilancookite.

Table 2. X-ray powder diffraction pattern of wilancookite.

I _{obs.}	d _{obs.}	I _{calc.}	$d_{\text{calc.}}$	hkl
10	9.77	63	9.602	110
60	6.90	60	6.790	200
80	5.54	53	5.544	211
5	4.84	13	4.801	220
40	4.53	_	_	_
_	_	33	4.294	301, 310
30	3.973	30	3.920	222
60	3.630	45	3.629	321, 312
20	3.351	1	3.395	400
70	3.212	66	3.201	330, 411
100	3.043	100	3.036	420,402
70	2.885	60	2.895	332
80	2.774	77	2.772	422
_	_	15	2.663	431, 501,
				510,413
30	2.485	32	2.479	512, 521
60	2.398	38	2.401	440
_	_	6	2.329	503, 530, 433
50	2.262	26	2.263	600,442
40	2.196	30	2.203	611, 523, 532
50	2.148	38	2.147	602,620
_	_	5	2.095	514,541
20	2.052	28	2.047	622
20	1.999	13	2.002	631,613

Data collected with a Gandolfi camera (diameter 114.6 mm), CuK α radiation (λ = 1.5418 Å) filtered with Ni. Intensities were estimated visually. The eight strongest lines are in bold. Calculated intensities were calculated from the structural data with POWDER CELL (Krauz & Nolze, 1996). Calculated *d* values were refined with LCLSQ (Burnham, 1991); the refined *a* value is 13.579(9) Å (space group *I*23).



Fig. 3. The crystal structure of wilancookite. The PO_4 tetrahedra are yellow, and the BeO_4 tetrahedra are blue. Green circles represent Ba atoms, and red circles O atoms and water molecules. (Online version in colour.)

were taken from the International Tables for X-ray Crystallography, Vol. C (Wilson, 1992). In the final refinement cycle, all atoms were refined anisotropically, leading to the R_1 value 0.0458. Further details on the crystal structure determination and refinement are given in Table 3; atomic coordinates, anisotropic displacement parameters, and bond lengths and angles are given in Tables 4–6, respectively.

Dimensions of	<i>ca.</i> $0.089 \times 0.070 \times 0.065$
the crystal (mm)	
a (Å)	13.5398(2)
$V(\dot{A}^3)$	2482.21(7)
Space group	<i>I</i> 23
Diffractometer	Rigaku XCalibur, EOS detector
Operating conditions	40 kV, 40 mA
Radiation	MoK α ($\lambda = 0.71073$ Å)
Scan mode	ϕ/ω scan
$2\theta_{\rm min}/2\theta_{\rm max}$	4.28°/57.14°
Range of indices	-7 < h < 17, -18 < k < 8,
6	-9 < l < 10
Measured intensities	1292
Unique reflections	805
Independent non-zero reflections	761 $[F_{\rm o} > 4\sigma(F_{\rm o})]$
Absorption correction	SCALE3 ABSPACK
1	(Agilent Technologies, 2012)
Structure solution program	SHELXS (Sheldrick, 2008)
L.s. refinement program	SHELXL (Sheldrick, 2008)
Refined parameters	73
$R_1 (F_0 > 4\sigma(F_0))$	0.0438
R_1 (all)	0.0458
wR_2 (all)	0.1357
S (goodness of fit)	1.149
Max Δ/σ in the	0.000
last l.s. cycle	
Max peak and hole in the final ΔF map (e/Å ³)	+1.17 and -0.65

Table 3. Experimental details for the single-crystal X-ray diffraction study of wilancookite.

The compatibility index of wilancookite was calculated with the relationship proposed by Mandarino (1981). The calculation of K_P was performed with the calculated density of 3.05 g/cm³. The compatibility index, $1 - (K_P/K_C)$, is 0.042, and ranges in the category "good" according to Mandarino (1981).

7. Discussion

a.,

The crystal structure of wilancookite is characterized by a framework similar to that of pahasapaite, $(Ca,Li,K,\square)_{24}$ $Li_8Be_{24}P_{24}O_{96}\cdot38H_2O$ (Rouse *et al.*, 1987, 1989). This framework is based on corner-sharing BeO₄ and PO₄ tetrahedra forming a large cavity in which occur Ba atoms and water molecules. As shown in Fig. 3, three different types of rings are building the cavity: eight-membered rings are parallel to (1 0 0) planes, six-membered rings are parallel to (1 1 1) planes, and four-membered rings are parallel to (1 1 0) planes. The positions of Ba atoms and water molecules are significantly different from those of Ca and Li in pahasapaite; however, the general topology of the framework is preserved.

Table	÷ 4.	Fina	1 fractional	coord	inates	and	equivalent	isotropic
displa	acen	nent p	parameters ($(Å^2)$ for	wiland	cooki	te.	

Site	x	у	Ζ	$U_{ m eq.}$
Ba1*	0	0.5	0.5	0.0270(4)
Ba2**	0.62566(7)	0.62566(7)	0.37434(7)	0.0323(6)
Р	0.8751(2)	0.7219(1)	0.4302(1)	0.0158(5)
Be	0.9303(7)	0.7729(8)	0.6245(8)	0.019(2)
01	0.8829(4)	0.6206(5)	0.3789(4)	0.022(1)
O2	0.8904(5)	0.6977(4)	0.5401(4)	0.021(1)
O3	0.7724(4)	0.7658(4)	0.4099(4)	0.018(1)
O4	0.9534(4)	0.7947(4)	0.3933(4)	0.020(1)
W1	0.434(1)	0.583(1)	0.282(1)	0.133(7)
W2	0.5	0.5	0.5	0.052(7)

Occupancy factors: *0.967(8) Ba + 0.033(8) \Box ; **0.532(6) Ba + 0.468(6) \Box .

The beryllophosphate tetrahedral framework of wilancookite is built by an array of truncated cubo-octahedral cages, linked together through octagonal prisms. In zeolite-RHO, the framework is undistorted, while in pahasapaite and wilancookite, both cages and octagonal prisms are strongly distorted (Fig. 4), thus leading to a symmetry reduction from *Im*3*m* to *I*23. This symmetry reduction is induced by the ordered distribution of Be and P on the tetrahedral sites of pahasapaite and wilancookite, while Al and Si are completely disordered on a single tetrahedral position in zeolite-RHO (Nenoff *et al.*, 1996; Rouse *et al.*, 1989).

The non-framework species in wilancookite are the Ba1 and Ba2 cations, as well as the W1 and W2 water molecules. These species are located in the cages, on different positions from those found in pahasapaite. The Ba1 atom is coordinated by twelve oxygens, with four short Ba1-O1 bonds of 2.807 Å, and eight long Ba1-O2 and Ba1-O4 bonds of 3.109-3.196 Å, respectively (Table 6). The Ba2 site is coordinated by three O3 atoms located at 2.790 Å, as well as by seven W1 and W2 water molecules located between 2.94 and 3.19 Å (Table 6). The morphologies of the Ba1 and Ba2 sites are compared in Fig. 5, where it appears that the Ba1 site corresponds to a fairly regular hexagonal prism, similar to that observed in minjiangite (Rao et al., 2015), whereas the Ba2 site is more irregular. Cationic distributions on these sites were calculated to reach a good agreement between the site scattering values given by the structure refinement (Table 4), and the chemical composition determined by electron microprobe (Table 1). According to these calculations, the Ba1 site is fully occupied by 94 at% Ba, 4 at% K and 2 at% Na, while the Ba2 site contains 52 at% Ba, 26 at% Li, and 22% vacancies.

The presence of Li on the Ba2 site affects its coordination polyhedron, which becomes more distorted, compared to the coordination polyhedron of the Ba1 site (Fig. 5). Moreover, the average Ba2–O bond distance (2.971 Å) is significantly shorter than the average Ba1–O bond distance (3.037 Å; Table 6), thus confirming the occurrence of Li on the Ba2 site. Lithium generally occurs in tetrahedral or octahedral coordinations (Wenger &

Site	U_{11}	U ₂₂	U_{33}	U ₂₃	<i>U</i> ₁₃	U_{12}
Ba1	0.0431(6)	0.0161(5)	0.0218(5)	0.000	0.000	0.000
Ba2	0.0323(6)	0.0323(6)	0.0323(6)	0.0045(4)	0.0045(4)	-0.0045(4)
Р	0.0139(9)	0.0171(9)	0.0164(9)	-0.0020(7)	0.0000(7)	0.0006(7)
Be	0.015(4)	0.025(5)	0.017(4)	-0.004(4)	0.000(4)	0.001(4)
01	0.026(3)	0.021(2)	0.020(2)	-0.004(2)	-0.004(2)	0.003(2)
02	0.027(3)	0.021(3)	0.016(2)	0.001(2)	0.000(2)	-0.009(2)
03	0.011(2)	0.015(3)	0.029(3)	-0.001(2)	0.002(2)	-0.004(2)
04	0.014(2)	0.023(3)	0.022(3)	0.001(2)	0.000(2)	0.001(2)
W1	0.15(2)	0.16(2)	0.085(9)	0.04(1)	-0.06(1)	-0.06(1)
W2	0.052(7)	0.052(7)	0.052(7)	0.000	0.000	0.000

Table 5. Anisotropic displacement parameters ($Å^2$) for wilancookite.

Table 6. Selected bond distances (Å) and angles (°) for wilancookite.

P01	1.542(5)	Ba1–O1 × 4	2.805(7)
PO2	1.536(6)	$Ba1-O2 \times 4$	3.109(6)
P-O3	1.537(6)	Ba1–O4 \times 4	3.196(6)
P04	1.531(6)	Mean	3.037
Mean	1.541		
Be-O1	1.595(12)	Ba2–O3 \times 3	2.790(5)
Be–O2	1.623(11)	$Ba2-W1 \times 3$	2.94(2)
Be–O3	1.630(12)	Ba2–W2	2.947(2)
Be–O4	1.621(11)	Ba2–W1′ \times 3	3.19(2)
Mean	1.617	Mean	2.971
O2-P-O1	103.7(3)	O1–Be–O2	112.1(7)
O2-P-O3	112.2(4)	O1–Be–O4	104.3(7)
O3-P-O1	109.0(3)	O2–Be–O3	110.4(7)
O4-P-O1	112.2(3)	O1–Be–O3	108.9(6)
O4–P–O2	111.1(3)	O4–Be–O2	109.4(7)
O4–P–O3	108.6(3)	O4–Be–O3	111.7(7)
Mean	109.5	Mean	109.5



Fig. 4. Comparison of the tetrahedral framework in zeolite-RHO (A – McCusker, 1984), in pahasapaite (B – Rouse *et al.*, 1987), and in wilancookite (C – this work). (Online version in colour.)



Fig. 5. Morphologies of the Ba1 (A) and Ba2 (B) sites of wilancookite. (Online version in colour.)

Armbruster, 1991); however, the presence of Li on larger crystallographic sites has been extensively demonstrated in synthetic alluaudite-type phosphates (Hatert *et al.*, 2000, 2002; Hatert, 2004; Trad *et al.*, 2010).

Wilancookite belongs to the pahasapaite group, Strunz 8.CA.25, Dana 40.5.7.1.; a comparison of the physical properties of wilancookite and pahasapaite is shown in Table 7. Wilancookite is only the second barium beryllophosphate reported to date, the first one being minjiangite (Rao *et al.*, 2015), a phyllophosphate characterized by a completely different structure topology.

Phase Reference	Wilancookite This work	Pahasapaite [1]
Ideal formula	(Ba,K,Na) ₈ (Ba,Li,□) ₆ Be ₂₄ P ₂₄ O ₉₆ ·32H ₂ O	(Ca,Li,K,□) ₂₄ Li ₈ Be ₂₄ P ₂₄ O ₉₆ ·38H ₂ O
Space group	<i>I</i> 23	I23
a (Å)	13.5398(2)	13.781(4)
Z	1	1
	9.77(10)	9.60(100)
	6.90(60)	_
	5.54(80)	5.61(30)
	_	4.35(40)
	3.630(60)	3.684(90)
Strong X-ray lines	3.212(70)	3.248(90)
	3.043(100)	3.081(30)
	2.885(70)	2.935(90)
	2.774(80)	2.702(60)
	2.398(60)	2.361(10)
Cleavage	None	None
Density	3.05 (calc.)	2.28
N	1.560(2)	1.523(2)
Hardness	4–5	4.5
Colour	Colourless	Colourless to light pink

Table 7. Comparison of the physical properties of wilancookite and pahasapaite.

[1] Rouse et al. (1987).

Wilancookite and pahasapaite are the only known phosphate minerals with a zeolite-type topology; however, synthetic beryllophosphates, zincophosphates and zincoarsenates with a zeolite topology were reported by Harvey (1988), Harvey & Meier (1989), Gier & Stucky (1991), and Harrison *et al.* (1991). Other zeolite minerals show a framework based on truncated cubo-octahedral cages connected by channels, as for example paulingite-Ca, (Ca,K,Na,Ba, \Box)₁₀(Si,Al)₄₂O₈₄·34H₂O (Lengauer *et al.*, 1997), and ashcroftine-(Y), K₅Na₅Y₁₂Si₂₈O₇₀(OH)₂ (CO₃)₈·8H₂O (Moore *et al.*, 1987).

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