THE CRYSTAL STRUCTURE OF BETPAKDALITE, AND A NEW CHEMICAL FORMULA: {Mg (H₂O)₆} Ca₂ (H₂O)₁₃ [Mo⁶⁺₈ As⁵⁺₂ Fe³⁺₃ O₃₆ (OH)] (H₂O)₄

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ABSTRACT

The crystal structure of betpakdalite, monoclinic, $C2/m$, a 19.531(2), b 11.061(1), c 15.257(2) Å, β 131.57(1)°, V 2466.6(5) Å³, $Z = 2$, has been refined to an R index of 2.5% for 3077 observed (5σ) reflections measured on a single crystal with Mo$K\alpha$ X-radiation. A crystal fragment was analyzed with an electron microprobe. Compared with previous work, the chemical analysis showed the absence of K and the presence of Mg. Moreover, the site assigned to K in previous work is far more stereochemically compatible with occupancy by Mg. The chemical formula of betpakdalite is redefined as {Mg (H₂O)₆} Ca₂ (H₂O)₁₃ [Mo⁶⁺₈ As⁵⁺₂ Fe³⁺₃ O₃₆ (OH)] (H₂O)₄.

Keywords: betpakdalite, crystal-structure refinement, electron-microprobe analysis, chemical formula.

SOMMAIRE

Nous avons affiné la structure cristalline de la betpakdalite, monoclinique, $C2/m$, a 19.531(2), b 11.061(1), c 15.257(2) Å, β 131.57(1)°, V 2466.6(5) Å³, $Z = 2$, jusqu'à un résidu R de 2.5% en utilisant 3077 réflexions observées (5σ), mesurées sur cristal unique avec rayonnement Mo$K\alpha$. Un fragment du même cristal a été analysé avec une microsonde électronique. Par rapport au travail antérieur effectué sur cette espèce, l'analyse chimique établit l'absence de l'potassium et la présence de magnésium. De plus, le site attribué au potassium dans le travail précédent est bien plus compatible avec la présence de magnésium selon les critères stéréochimiques. La formule chimique de la betpakdalite serait {Mg (H₂O)₆} Ca₂ (H₂O)₁₃ [Mo⁶⁺₈ As⁵⁺₂ Fe³⁺₃ O₃₆ (OH)] (H₂O)₄.

(Traduit par la Rédaction)

Mots-clés: betpakdalite, affinement de la structure cristalline, analyse à la microsonde électronique, formule chimique.

INTRODUCTION

Betpakdalite was first described by Ermilova & Senderova (1961). It was later discovered at the Tsumeb mine, Namibia, and the crystal structure of a sample from this locality was reported by Schmetzer *et al.* (1984). Detailed electron-microprobe compositions were also given by Schmetzer *et al.* (1984), who reported the chemical formula as H₆₋ₓ [K (H₂O)₆]ₓ [Ca (H₂O)₆]₄ [Mo₁₆ As₄ Fe₆ O₇₄] •4H₂O. However, disorder between H and [K (H₂O)₆] seems unlikely, and the [K(H₂O)₆] octahedron had a mean bond-length of 2.18 Å, which is unrealistically short for a K–(H₂O) bond. Moore (1992) presented a detailed analysis of the betpakdalite structure, based on the results of Schmetzer *et al.* (1984), and commented on the unlikely assignment of K in the structure. We had the opportunity to acquire excellent crystals of betpakdalite, and did so in order to resolve this problem.

EXPERIMENTAL

Data collection

Exceptional crystals of betpakdalite were provided to us by Mr. William W. Pinch of Rochester, New York. The sample consists of bright yellow crystals of betpakdalite embedded in and perched on greyish green scorodite from the Tsumeb mine, Namibia, similar to the material examined by Schmetzer *et al.* (1984). An equant crystal was mounted on a Siemens *P*4 automated four-circle diffractometer and aligned on thirty relatively intense reflections; the cell dimensions (Table 1) were determined by least-squares refinement of the resultant setting angles. A total of 5230 reflections was collected out to 60°2θ over the index ranges $\overline{27} \le h \le 22$, $\overline{2} \le k \le 15$, $\overline{2} \le l \le 16$ with scan speeds between 1.33 and 5.00°2θ/min. A total of 1980 psi-scan intensities were collected for 33 reflections at intervals of 6° about

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TABLE 1. MISCELLANEOUS INFORMATION FOR BETPAKDALITE

a (Å)	19.531(2)	crystal size (mm)	0.06 x 0.10 x 0.12
b	11.061(1)	Radiation	Mo$K\alpha$/Graphite
c	15.257(2)	Total no. of I	5230
β (°)	131.57(1)	No. of $|F|$	3791
V (Å^3)	2466.6(5)	R(merge) %	1.3
Sp Gr.	$C2/m$	No. of $|F_o| > 5\sigma$	3077
Z	2	R(azimuthal) %	1.9 → 1.0
		R (obs) %	2.5
		wR (obs) %	2.7

Unit formula: {Mg (H$_2$O)$_6$} Ca$_2$ (H$_2$O)$_{13}$ [Mo$_8^{6+}$ As$_2^{5+}$ Fe$_3^{3+}$ O$_{36}$ (OH)] (H$_2$O)$_4$

$R = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|$

$wR = [\Sigma w(|F_o| - |F_c|)^2/\Sigma F_o^2]^{\frac{1}{2}}$, $w = 1$

the diffraction vector, and subsequent absorption correction reduced R(azimuthal) from 1.9% to 1.0%. The normal intensity data were then corrected for absorption, Lorentz, polarization and background effects, averaged and reduced to structure factors; of the 3791 unique reflections, 3077 were considered as observed ($F_o > 5\sigma F$).

A cleavage fragment of betpakdalite was attached to a plexiglass disk, carbon coated and analyzed with a Cameca SX–50 electron microprobe operating in wavelength-dispersion mode with the following conditions: excitation voltage 15 kV, beam current 20 nA, peak count-time 20 s, background count-time 10 s, beam size 10 μm. The following standards were used; molybdenite: Mo, forsterite: Mg, diopside: Ca, cobaltite: As, and fayalite: Fe; in addition, K and F were sought but not detected. Data reduction was done with the $\phi(\rho z)$ procedure of Pouchou & Pichoir (1985). The formula was calculated on the basis of 60 anions including 23 (H$_2$O) groups and 1 (OH) group. The chemical composition and unit formula are reported in Table 2.

Crystal-structure refinement

All calculations were done with the SHELXTL PC Plus system of programs; R and wR indices are of the form given in Table 1, and are expressed as percentages. The structure model of Schmetzer *et al.* (1984) was used as a starting model with the exception that K was replaced by Mg at the $Mg(K)$ site. The structure converged rapidly, but there were several unsatisfactory aspects to the refined model:

(1) Schmetzer *et al.* (1984) reported the $W(1)$ site as two-thirds occupied (which they forced to agree with the two-thirds occupancy of their K site); however, this site refines satisfactorily when fully occupied, and gives reasonable displacement-factors.

(2) The $W(5)$ site was reported as fully occupied on the position (x 0 z), but with a very high displacement-parameter; a more satisfactory model is obtained if the $W(5)$ site is disordered to the general position (x y z) with half-occupancy.

(3) The $W(8)$ site was reported as half-occupied; refinement of the occupancy of this site converged to 1.05(2). The equivalent isotropic-displacement parameter is high (Table 2), but the site is definitely filled.

(4) A new position $W(10)$, was found in the present refinement; it is one-quarter occupied by O ($\equiv$ H$_2$O).

(5) The O(12) site was reported as being on the mirror plane, but had a large displacement parameter; a more satisfactory model is obtained if the site is disordered off the mirror plane.

With these changes, the refinement converged to an R index of 2.5%. Final parameters are listed in Table 3, and selected interatomic distances are given in Table 4. Bond valences were calculated with the parameters of Brown & Altermatt (1985) and are given in Table 5. Observed and calculated structure-factors may be obtained from The Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2.

DISCUSSION

The topology of the betpakdalite structure was discussed in detail by Moore (1992), who showed that it is close-packed with a large proportion of vacancies substituted for anions. Thus our discussion here will focus on crystal-chemical aspects of betpakdalite.

The Mg site

Schmetzer *et al.* (1984) reported a two-thirds-occupied K site coordinated by six (H$_2$O) groups, with a $\langle K-$(H$_2$O)$\rangle$ distance of 2.18 Å. The ionic radii of Shannon (1976) predict a $\langle^{[6]}$K–O$\rangle$ distance of 1.38 + 1.36 = 2.74 Å, in complete disagreement with the observed $\langle K-$(H$_2$O)$\rangle$ distance of 2.18 Å. Schmetzer *et al.* (1984) reported K$_2$O contents in the range 0.51–3.52 wt.% in betpakdalite; however, we did not detect K in our electron-microprobe work. However, we did detect the presence of significant Mg (Table 2). Moreover, calculation of the unit formula of betpakdalite from the chemical composition gives 1.0 Mg *apfu* (atoms per formula unit). This amount of Mg will completely fill the K site of

TABLE 2. CHEMICAL COMPOSITION* (wt.%) AND UNIT FORMULA (*apfu*) FOR BETPAKDALITE

MgO	1.8	Mg	1.0
CaO	5.3	Ca	2.1
MoO$_3$	52.9	Mo	8.0
As$_2$O$_5$	10.0	As	1.9
Fe$_2$O$_3$	11.2	Fe	3.1
H$_2$O	(19.4)		
Total	100.6	H$_2$O	23
		OH	1

* not detected: K, F

TABLE 3. ATOMIC POSITIONS AND DISPLACEMENT PARAMETERS* FOR BETPAKDALITE

Site	**s.o.	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
Mo(1)		0.21480(2)	−0.16070(3)	0.19391(2)	99(1)	75(1)	86(1)	7(1)	69(1)	8(1)	81(1)
Mo(2)		0.37106(3)	0	0.19692(3)	76(2)	82(2)	81(2)	0	53(2)	0	79(2)
Mo(3)		0.37566(3)	0	0.42461(4)	96(2)	178(2)	83(2)	0	58(2)	0	120(2)
As		−0.13451(3)	0	0.05884(4)	83(2)	85(2)	84(2)	0	57(2)	0	83(2)
Fe(1)		3/4	3/4	0	127(3)	94(3)	127(3)	9(3)	90(3)	−4(3)	111(4)
Fe(2)		0	0	0	109(4)	142(5)	130(5)	0	91(4)	0	119(5)
Mg		1/2	0	0	172(13)	270(16)	244(14)	0	143(12)	0	224(16)
Ca	0.5	0.1559(1)	−0.1768(2)	0.4880(2)	336(10)	261(10)	302(9)	115(8)	172(8)	−5(8)	330(11)
O(1)		0.2126(2)	0	0.0926(2)	102(15)	88(16)	76(15)	0	51(13)	0	94(17)
O(2)		0.2375(2)	0	0.2852(3)	111(16)	131(17)	116(16)	0	81(14)	0	115(18)
O(3)		0.3423(2)	−0.1249(6)	0.1022(2)	162(12)	133(12)	188(13)	−35(10)	125(11)	−16(10)	153(14)
O(4)		0.3505(2)	−0.1137(3)	0.2869(2)	133(11)	162(12)	132(11)	1(10)	98(10)	5(10)	135(13)
O(5)		0.2184(2)	−0.2546(3)	0.1012(2)	211(13)	131(12)	196(12)	−22(10)	168(11)	−15(10)	153(14)
O(6)		0.0947(2)	−0.1279(3)	0.1007(2)	140(12)	158(13)	167(12)	7(10)	103(11)	7(10)	154(14)
O(7)		0.1513(2)	−0.1243(3)	−0.1056(2)	223(13)	142(13)	109(11)	−19(10)	92(11)	61(11)	173(14)
O(8)		0.0285(2)	0	−0.1066(3)	77(16)	335(23)	110(16)	0	66(14)	0	171(19)
O(9)		0.3708(2)	−0.1229(3)	0.4889(3)	233(14)	252(16)	155(13)	23(12)	104(12)	−26(12)	233(16)
O(10)		0.4873(3)	0	0.2926(3)	124(17)	249(21)	134(17)	0	76(15)	0	176(20)
O(11)		0.2346(2)	−0.2608(3)	0.2940(3)	255(14)	192(14)	170(13)	50(11)	151(12)	29(12)	197(15)
O(12)	0.5	1/2	0.014(5)	1/2	80(24)	314(199)	151(26)	0	69(22)	0	188(72)
W(1)		0.4657(3)	−0.1347(5)	0.0586(4)	370(20)	641(30)	462(23)	2(21)	286(19)	−199(21)	483(26)
W(2)		0.6294(3)	0	0.1650(5)	230(24)	528(35)	335(27)	0	146(23)	0	397(30)
W(3)		−0.2077(4)	0	0.2216(5)	535(34)	400(31)	459(32)	0	405(30)	0	405(38)
W(4)	0.5	0.1277(5)	−0.0504(7)	0.3390(6)	318(34)	602(49)	240(31)	125(31)	208(29)	59(32)	368(39)
W(5)	0.5	−0.1056(7)	−0.030(1)	0.4644(8)	716(60)	676(113)	577(53)	54(50)	376(49)	−145(55)	698(72)
W(6)	0.5	−0.2951(5)	−0.0419(6)	0.4039(6)	370(35)	279(32)	386(36)	−7(27)	284(32)	32(27)	319(41)
W(7)	0.5	−0.2335(6)	−0.2001(6)	0.5028(7)	656(54)	251(34)	475(41)	10(33)	471(43)	84(36)	385(54)
W(8)		0.4798(5)	−0.3068(6)	0.3544(6)	738(42)	658(42)	1078(54)	−224(40)	110(39)	163(35)	1214(53)
W(9)	0.5	0.0569(6)	−0.2307(9)	0.2597(8)	446(49)	429(52)	558(55)	11(45)	258(45)	−13(43)	537(59)
W(10)	0.25	0.417(1)	−0.200(2)	0.702(2)	–	–	–	–	–	–	494(43)

* $U \times 10^4$; **s.o.: site-occupancy, not given if 1.0.

Schmetzer *et al.* (1984), and is more in accord with the observed scattering power at this site and with the reported mean bond-length of 2.18 Å. Insertion of Mg at the *K* site resulted in a well-behaved refinement, a reasonable value for the displacement factor at this site, and an observed mean bond-length (2.066 Å) that is in accord with the assigned occupancy; hence this site was relabeled *Mg* and considered to be completely occupied by Mg.

The structural unit

Schmetzer *et al.* (1984) wrote the structural unit of betpakdalite as $[Mo^{6+}_{16} As^{5+}_4 Fe^{3+}_6 O_{74}]$, which can be reduced to $[Mo^{6+}_8 As^{5+}_2 Fe^{3+}_3 O_{37}]$. The present refinement gave the same cation and anion proportions, but the resulting complete formula, $\{Mg (H_2O)_6\} Ca_2 (H_2O)_{13} [Mo^{6+}_8 As^{5+}_2 Fe^{3+}_3 O_{37}] (H_2O)_4$ has an excess negative charge of 1^-. Careful inspection of the local environment of each anion, together with the bond-valences (Table 5), indicates that there is an additional

H-atom in the structure. In this regard, the newly identified partly occupied $W(10)$ site is adjacent to the $O(10)$ site, which is bonded to a Mo^{6+} cation. The $O(10)$ site is bonded *only* to Mo^{6+} at the $Mo(2)$ site and receives an incident bond-valence of only 1.75 valence units, *vu* (Table 5). Moreover, the nearest *W* site is 3.46 Å away from O(10), and hence the latter cannot act as an acceptor for a H-bond. These factors suggest two local (short-range) environments (Fig. 1). In the first local arrangement, O^{2-} at O(10) has a short bond (~1.65 Å) to $Mo(2)$, and its bond-valence requirements are completely satisfied by the single $Mo(2)$–O(10) bond; note that the adjacent $W(10)$ site is vacant. In the second local arrangement, $(OH)^-$ at O(10) has a longer bond (~1.80 Å) to $Mo(2)$, which contributes a bond-valence of ~1.34 *vu*. The O(10)–H bond-valence of ~0.80 *vu* results in an H-bond from O(10) [= OH] to $W(10)$, which is occupied by (H_2O) in this configuration. Thus the composition of O(10) is $O_{0.5}(OH)_{0.5}$, and the observed average incident bond-valence at O(10) [solely from $Mo(2)$] is $(2.00 + 1.34)/2 \approx 1.67$ *vu*, which is close to

TABLE 4. SELECTED INTERATOMIC DISTANCES (Å) FOR BETPAKDALITE

Mo(1)–O(1)	2.337(4)		Fe(1)–O(3)b,d	1.966(2)	x2
Mo(1)–O(2)	2.116(3)		Fe(1)–O(5)b,d	2.008(5)	x2
Mo(1)–O(4)	2.078(3)		Fe(1)–O(7)b,d	2.030(3)	x2
Mo(1)–O(5)	1.793(4)		<Fe(1)–O>	2.001	
Mo(1)–O(6)	1.798(3)				
Mo(1)–O(11)	1.710(4)		Fe(2)–O(6),a,c,e	2.003(2)	x4
<Mo(1)–O>	1.972		Fe(2)–O(8),a	2.038(6)	x2
			<Fe(2)–O>	2.015	
Mo(2)–O(1)	2.361(4)				
Mo(2)–O(3),c	1.799(3)	x2	Mg–W(1),c,g,h	2.065(6)	x4
Mo(2)–O(4),c	2.088(4)	x2	Mg–W(2),h	2.069(4)	x2
Mo(2)–O(10)	1.699(4)		<Mg–W>	2.066	
<Mo(2)–O>	1.972				
			Ca–O(9)f	2.356(4)	
Mo(3)–O(2)	2.047(3)		Ca–O(11)f	2.583(4)	
Mo(3)–O(4),c	2.206(3)	x2	Ca–W(4)	2.401(10)	
Mo(3)–O(9),c	1.715(4)	x2	Ca–W(5)l	2.254(15)	
Mo(3)–O(12)	1.881(4)		Ca–W(6)i	2.527(8)	
<Mo(3)–O>	1.962		Ca–W(7)j	2.435(12)	
			Ca–W(8)k	2.590(8)	
As–O(1)a	1.728(3)		Ca–W(9)	2.700(11)	x½
As–O(7)a,e	1.679(4)	x2	Ca–W(10)f	2.611(22)	x½
As–O(8)a	1.679(5)		<Ca–φ>	2.460	
<As–O>	1.691				
W(4)–W(4)c	1.11(2)		W(6)–W(7)	2.09(1)	
W(4)–W(9)	2.27(1)		W(7)–W(7)l	1.25(2)	
W(5)–W(5)c	0.66(2)		Ca–W(7)i	1.45(1)	
W(6)–W(6)c	0.93(1)		W(9)–W(10)f	0.90(2)	
			O(10)......W(10)m	2.86(3)	

a: $\bar{x}$, y, $\bar{z}$; b: $\bar{x}$+1, y+1, $\bar{z}$; c: x, $\bar{y}$, z; d: x+½, $\bar{y}$+½, z; e: $\bar{x}$, $\bar{y}$, $\bar{z}$; f: $\bar{x}$+½, $\bar{y}$–½, $\bar{z}$+1; g: $\bar{x}$+1, $\bar{y}$, $\bar{z}$; h: $\bar{x}$+1, y, $\bar{z}$; i: $\bar{x}$, y, $\bar{z}$+1; j: x+½, $\bar{y}$–½, z; k: x–½, $\bar{y}$–½, z; l: $\bar{x}$–½, $\bar{y}$–½, $\bar{z}$+1; m: $\bar{x}$+1, y, $\bar{z}$+1

TABLE 5. BOND-VALENCE (vu) TABLE FOR BETPAKDALITE

	Mo(1)	Mo(2)	Mo(3)	As	Fe(1)	Fe(2)	Mg	Ca	Σ
O(1)	0.31^{x2}~	0.29		1.11					2.02
O(2)	0.57^{x2}~		0.68						1.82
O(3)		1.34^{x2}↓			0.55^{x2}↓				1.89
O(4)	0.63	0.61^{x2}↓	0.45^{x2}↓						1.69
O(5)	1.36				0.49^{x2}↓				1.85
O(6)	1.34					0.50^{x4}↓			1.84
O(7)				1.27^{x2}↓	0.47^{x2}↓				1.74
O(8)				1.27		0.46^{x2}↓			1.73
O(9)			1.68^{x2}↓					0.35^{x½}~	1.86
O(10)		1.75							1.75
O(11)	1.70							0.19^{x½}↓	1.80
O(12)			1.07^{x2}~						2.14
W(1)							0.35^{x4}↓		0.35
W(2)							0.35^{x2}↓		0.35
W(3)									0.00
W(4)								0.31	0.31
W(5)								0.46	0.46
W(6)								0.22	0.22
W(7)								0.28	0.28
W(8)								0.19^{x½}~	0.10
W(9)									0.00
W(10)								0.18^{x½}↓	0.18
Σ	5.91	5.94	6.01	4.92	3.02	2.92	2.10	2.09	

the observed value of 1.75 *vu* (Table 5). This model results in a change in the structural unit: $[Mo^{6+}_8 As^{5+}_2 Fe^{3+}_3 O_{36} (OH)]$, and a neutral chemical formula.
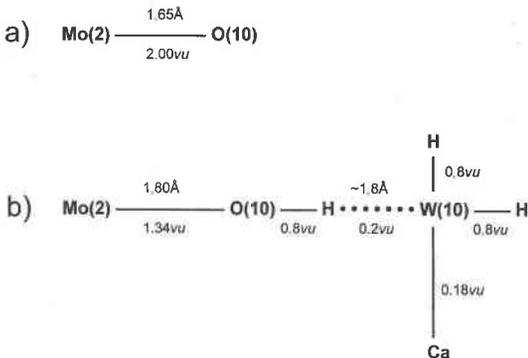

Fig. 1. Alternative configurations involving the Mo(2)–O(10) bond in betpakdalite: (a) [1]- coordinated O(10) anion [= O^{2-}]; (b) [2]-coordinated O(10) anion [= OH⁻].

Coordination of the Ca site

The *Ca* site is exactly half-occupied by Ca. Schmetzer *et al.* (1984) reported Ca as [8]-coordinated by O(9), O(11), and six (H_2O) groups. However, the situation must be more complicated than this at the local scale; at some of the anion sites, only half of the anions are bonded to Ca, and hence there must be significant relaxation to satisfy the local anion bond-valence requirements of the anions. As noted in Table 4, *Ca* is adjacent to two O-atoms and seven *W* sites. However, some of the *W* sites are only half-occupied, and one [*W*(10)] is one-quarter occupied. The Ca–φ interatomic distances that correspond to Ca–φ bonds are shown in bold font in Table 4; Ca is both [7]- and [8]-coordinated.

A scheme of local order between neighboring Ca polyhedra and flanking *Mo*(2) octahedra is presented in Figure 2. Four Ca sites are shown, *Caa* and *Cac* are occupied, and *Cab* and *Cad* are vacant. The anions at O(9), O(11) and *W*(8) have the same multiplicity as *Ca*, but they are fully occupied sites, and therefore must relax their positions (or receive H-bonds, or both) where the neighboring *Ca* site is vacant. The H_2O groups at *W*(4), *W*(5), *W*(6), *W*(7) and *W*(9) have the same multiplicity and the same occupancy as the *Ca* site. Occupancy of a *Ca* site (*Caa*, *Cac*) is associated with occupancy of the coordinated *W*(4), *W*(5), *W*(6) and *W*(7) sites, and vacancy at the *W*(9) site. The vacancy at the *W*(9) site occurs because the *W*(4) and *W*(9) sites are too close together [2.27(1) Å] to be simultaneously occupied. The *Ca–W*(4) bond of 0.31 *vu* is deemed an essential contribution to the bond-valence sum at *Ca*. There is another close approach between adjacent *W*(9) and *W*(10) sites [0.90(2) Å]. As a result, *W*(9) never
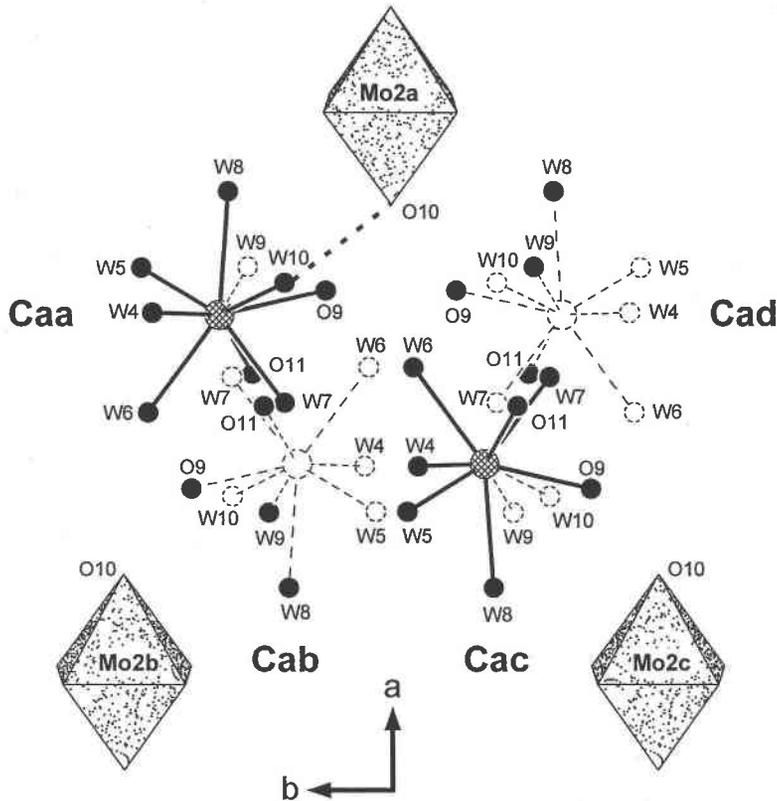
FIG. 2.   Scheme of local order involving *Ca* sites in betpakdalite; filled (shaded) circles are occupied sites, unshaded broken circles are vacant sites, full lines show chemical bonds, broken lines show nearest-neighbor sites in which at least one site is not occupied. The *Ca* sites are labeled *a* (= *Caa*), *b*, *c* and *d* for ease of identification in the text.

bonds to *Ca*, and *W*(10) is always bonded to *Ca*. Because the occupancy factor for the *W*(10) site and *Ca* site is ¼ and ½, respectively, only half the *Ca* sites will be coordinated by an H_2O group at *W*(10). Half of the occupied *Ca* sites in betpakdalite are therefore [8]-coordinated (*Caa*), and the other half are [7]-coordinated (*Cac*). Where the *W*(10) site is occupied by an H_2O group (*Caa* polyhedron), it receives a H-bond from the nearby OH group at the *O*(10) site. Can two neighboring *Ca* sites (*i.e.*, *Caa* and *Cab*) both be occupied? No, the H_2O group at *W*(7) is bonded to *Caa* and lies 1.45(1) Å from *Cab*; this precludes Ca occupation of *Cab*. The *W*(10) site associated with the occupied *Cac* site is shown as vacant; however, it could have been shown as occupied, the only stipulation being that one half of the occupied *Ca* sites overall must be associated with vacant *W*(10) sites.

CONCLUSION

The chemical formula of betpakdalite is as follows:

{Mg ($H_2O)_6$} Ca_2 ($H_2O)_{13}$
[Mo^{6+}_8 As^{5+}_2 Fe^{3+}_3 O_{36} (OH)] ($H_2O)_4$
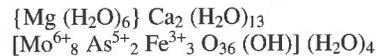
where (H_2O) groups placed before the structural unit are bonded directly to interstitial cations and (H_2O) groups placed after the structural unit are held in the structure only *via* H-bonding.

ACKNOWLEDGEMENTS

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