Mineralogical Magazine, August 2018, Vol. 82(4), pp. 929–937

Chemographic exploration of the hyalotekite structure-type

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[*Received 23 July 2017; Accepted 19 September 2017; Associate Editor: G. Diego Gatta*]

ABSTRACT

The hyalotekite group has been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (memorandum 57–SM/16). The general formula of the minerals of the hyalotekite group may be written as: $A_2B_2M_2[Si_8T_4O_{28}]W$ where A = Ba^{2+}, Pb^{2+} or K^+; B = Ba^{2+}, Pb^{2+} or K^+; M = Ca^{2+}, Y^{3+} or REE^{3+}; T = Si^{4+}, B^{3+} or Be^{2+}; and W = F^- or □ (where *REE* = rare-earth elements and □ = vacancy).

Four minerals are currently known in this group: hyalotekite, $Ba_4Ca_2[Si_8B_2(SiB)O_{28}]F$, triclinic, $I\bar{1}$; khvorovite, $Pb^{2+}_4Ca_2[Si_8B_2(SiB)O_{28}]F$, triclinic $I\bar{1}$; kapitsaite-(Y), $Ba_4(YCa)[Si_8B_2B_2O_{28}]F$, triclinic, $I\bar{1}$; and itsiite $Ba_4Ca_2[Si_8B_4O_{28}]$□, tetragonal, $I\bar{4}2m$.

We explore the possible end-member compositions within this group by conflating the properties of an end-member with the stoichiometry imposed by the bond topology of the hyalotekite structure-type and the crystal-chemical properties of its known constituents. There are two high-coordination sites in the hyalotekite structure, *A* and *B*, and occupancy of each of these sites can be determined only by crystal-structure refinement. If these two sites are considered together, there are 19 end-member compositions of the triclinic structure and six end-member compositions of the tetragonal structure involving A and B = Ba^{2+}, Pb^{2+}, K^+; M = Ca^{2+}, Y^{3+}, REE^{3+}; and T = Si^{4+}, B^{3+}, Be^{2+}. There is the possibility for many other hyalotekite-group minerals, and two potential new minerals have been identified from data in the literature.

Keywords: hyalotekite group, chemographic exploration, end-members, hyalotekite, khvorovite, kapitsaite-(Y), itsiite.

Introduction

Nordenskiöld (1877) described hyalotekite as a new Pb-silicate mineral from Långban, Värmland, Sweden. A more comprehensive chemical analysis of holotype material was given by Lindström (1887), showing the presence of Ba, Pb, Be and B, and both analyses of holotype hyalotekite show Ba in excess of Pb (Table 1). Based on the chemical analysis of Lindström (1887) and calculated on 29 (O + F) anions, the empirical formula of hyalotekite from Långban is $(Ba_{1.96}Pb^{2+}_{1.68}K_{0.28}Na_{0.08})_{\Sigma4}(Ca_{2.08}Mn_{0.06}Mg_{0.03}Cu_{0.02})_{\Sigma2.19}(Si_{9.82}B_{1.60}Be_{0.45}Al_{0.05}Fe^{3+}_{0.01})_{\Sigma11.93}O_{28.20}F_{0.78}Cl_{0.03}$ for $Z = 2$. The general formula has been written in various ways (Moore *et al.*, 1982; Grew *et al.*, 1994, Christy *et al.*, 1998), and the currently accepted form is as follows: $(Ba,Pb^{2+},K)_4(Ca,Y)_2[Si_8(B,Be)_2(Si,B)_2O_{28}]F$ (Pautov *et al.*, 2015). Hyalotekite has been reported from the Darai-Pioz alkaline massif, Tajikistan (Grew *et al.*, 1994). Two other minerals isostructural with hyalotekite have also been reported from the Darai-Pioz massif: kapitsaite-(Y), ideally $Ba_4(YCa)[Si_8B_2B_2O_{28}]F$ (Pautov *et al.*, 2000; Sokolova *et al.*, 2000) and khvorovite, ideally $Pb^{2+}_4Ca_2[Si_8B_2(SiB)O_{28}]F$ (Pautov *et al.*, 2015). The degree of complication of the hyalotekite structure, combined with the complexity of the parageneses in which it has been found, suggest the possibility of: (1) the occurrence of additional

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https://doi.org/10.1180/minmag.2017.081.076

TABLE 1. Crystallographic data for the hyalotekite-group minerals.

	Hyalotekite $Ba_4Ca_2[Si_8B_2(SiB)O_{28}]F$	Khvorovite $Pb^{2+}_4Ca_2[Si_8B_2(SiB)O_{28}]F$	Kapitsaite-(Y) $Ba_4(YCa)[Si_8B_2B_2O_{28}]F$	Itsiite $Ba_4Ca_2[Si_8B_4O_{28}]\square$
a (Å)	11.310(2)	11.354(2)	11.181(4)	10.9515(5)
b (Å)	10.955(2)	10.960(2)	10.850(7)	10.9515(5)
c (Å)	10.317(3)	10.271(2)	10.252(4)	10.3038(7)
α (°)	90.43(2)	90.32(3)	90.64(6)	90
β (°)	90.02(2)	90.00(3)	90.05(4)	90
γ (°)	90.16(2)	90.00(3)	89.97(7)	90
V (Å)^3	1278.2	1278(1)	1243.6(9)	1235.79(11)
Space group	$I\bar{1}$	$I\bar{1}$	$I\bar{1}$	$I\bar{4}2m$
Z	2	2	2	2
Reference	(1)	(2)	(3)	(4)

References: (1) Moore *et al.* (1982); (2) Pautov *et al.* (2015); (3) Sokolova *et al.* (2000); (4) Kampf *et al.* (2014).

hitherto-undiscovered minerals; and (2) the possibility of synthesizing a wide variety of chemical variants. These points have encouraged us to define the Hyalotekite Group, approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA) in memorandum 57–SM/16, and to examine the hyalotekite structure-type in terms of its possible chemical variants.

End-members and their significance

From an algebraic perspective, a 'chemical system' is described in terms of its components. 'System components' are those (components) required to describe the chemical variability of the system, and 'phase components' are those components required to describe the chemical variability in individual phases (Spear, 1993). Phase components must be independently variable (Gibbs, 1961), i.e. they must be additive, and for minerals, they must be conformable with the structure of that mineral. If we define our system as conforming to a specific structure type, we may define the components of this system as the smallest set of chemical formulae required to describe the composition of all minerals in the system. The definition, 'the smallest set of chemical formulae required to describe the composition of all the phases in the system', defines the components of the system as its set of end-member compositions, and the set of end-member compositions define the possible composition space occupied by that structure type. These components have certain constraints (Hawthorne, 2002): (1) they must be conformable with the structure type of the mineral; (2) they must be neutral (i.e. not carry an electric charge); and (3) they must be irreducible within the system considered (i.e. they cannot be expressed as two or more simpler compositions that are compatible with the crystal structure of the system).

For the majority of atomic arrangements and chemical compositions, these constraints result in end-member formulae which have a single constituent at each site [e.g. diopside: $CaMgSi_2O_6$: $M(1) = Mg^{2+}$, $M(2) = Ca^{2+}$, $T = Si^{4+}$, $O(1) = O(2) = O(3) = O^{2-}$] or group of sites (forsterite: Mg_2SiO_4: $M(1) + M(2) = Mg^{2+}$, $T = Si^{4+}$, $O(1) = O(2) = O(3) = O(4) = O^{2-}$] in the structure. However, Hawthorne (2002) showed that some end-members have two constituents of different valence and in a fixed ratio at one site in their structure (the remaining sites having only one constituent each). A classic example of this is milarite, $K_2Ca[AlBe_2Si_{12}O_{30}](H_2O)$, in which $T(2) = Be_2Al$ apfu (atoms per formula unit) in the end-member formula. Note that an end-member can have more than one species at only one site, and only two species at that site. If more than one cation or anion is introduced to another site in the structure, or a third species is introduced to a site, the resulting composition is reducible and may be resolved into two end-member compositions.

The hyalotekite-type structure

The crystal structure of hyalotekite was solved by Moore *et al.* (1982) and refined (using the same diffraction data) by Christy *et al.* (1998). The structure consists of layers of corner-sharing (SiO_4) tetrahedra interleaved with layers of (TO_4) tetrahedra and Ba^{2+}

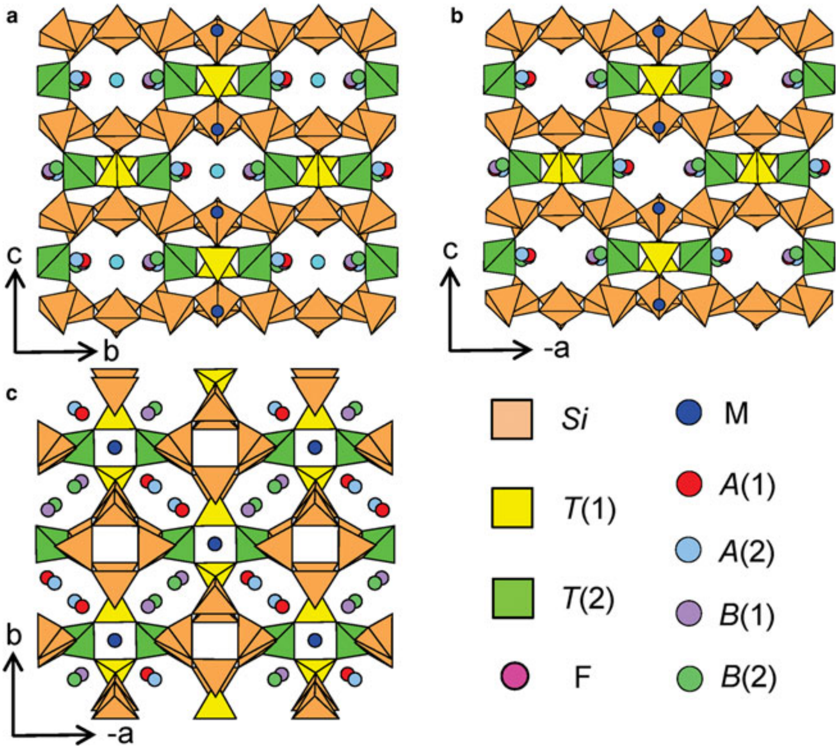

FIG. 1. The crystal structure of hyalotekite; (*a*) viewed down **a**; (*b*) viewed down **b**; (*c*) viewed along **c**; the *W* site is concealed behind the *M* site in (*c*).

(Figs 1*a*,*b*), forming an interrupted framework of corner-shared *Si*, *B* and *T* tetrahedra with interstitial Ba^{2+} and Ca^{2+} in the channels through the framework. There are four [4]-coordinated *Si* sites occupied solely by Si^{4+}, giving Si_8 apfu. Previous crystal-structure work on hyalotekite-group minerals (e.g. Sokolova *et al.*, 2000; Pautov *et al.*, 2015) identified two distinct tetrahedrally coordinated sites, *B* occupied solely by B^{3+}, and *T* occupied by B^{3+} and Si^{4+}. As we shall show later, the *B* site in other potential hyalotekite-group minerals may be occupied by cations other than B^{3+}, and hence we relabel the *B* and *T* sites as *T*(1) and *T*(2). In hyalotekite, *T*(1) is occupied by B^{3+} and *T*(2) is occupied by B^{3+} and Si^{4+}, giving ideally (SiB_3) apfu. The *Si*(1–4) tetrahedra form four-membered $[Si_4O_{12}]$ rings (Fig. 1*c*), and the *T* tetrahedra form four-membered $[T_4O_{12}]$ rings. Tetrahedra of both rings share vertices to form an interrupted $[Si_8T_4O_{28}]$ framework of ideal composition $[Si_8B_2(SiB)O_{28}]$ apfu in hyalotekite itself.

There are two interstitial sites that have been labelled *A*(1) and *A*(2) in previous work. Each of these sites splits into two subsites, ~0.5 Å apart: *A*(1) = *A*(11) + *A*(12) and *A*(2) = *A*(21) + *A*(22). We will simplify this site nomenclature by designating *A*(1) as *A* and *A*(2) as *B*; the split sites then become *A*(1) + *A*(2), with coordination numbers [8] and [9], and *B*(1) + *B*(2), with coordination numbers [8] and [10]. The *A* and *B* sites are occupied by Pb^{2+}, Ba^{2+}, K^+ and minor Na^+, and their ideal composition in hyalotekite is Ba_4 apfu (Table 1). There is one interstitial [8]-coordinated *M* site that is occupied by Ca^{2+} in hyalotekite, with the ideal composition Ca_2 apfu.

There are 15 anion sites in the structure. Ten O^{2-} anions bridge tetrahedra of the interrupted framework, and three O^{2-} anions are each bonded to one Si^{4+} cation atom and to three interstitial cations. There is one monovalent-anion site that is coordinated by two *M* (= Ca^{2+}) and four *A* cations, and it is occupied by F^-.

The bond-valence table for khvorovite is shown as Table 2. There are several features of interest here. First, note that the *W* site is surrounded by two *A*, two *B* and two *M* cation sites, and hence the F^- ion at the *W* site is octahedrally coordinated by cations at the locally associated cation sites. This

TABLE 2. Bond-valence* table for khvorovite.

	A(1)	*A*(2)	*B*(1)	*B*(2)	*M*	*T*	*B*	*Si*(1)	*Si*(2)	*Si*(3)	*Si*(4)	Σ
O(1)	0.04	0.034							0.97		1.02	2.06
O(2)			0.02	0.04					1.01	1.09		2.16
O(3)	0.03	0.02						1.05		0.92		2.02
O(4)			0.05	0.06				1.06			1.01	2.18
O(5)			0.06	0.11		0.92		0.92				2.02
O(6)	0.17	0.06				0.87			1.01			2.11
O(7)				0.05	0.32	0.90	0.70					1.97
O(8)		0.02			0.30	0.96	0.70					1.98
O(9)				0.02			0.82			1.04		1.88
O(10)					0.31		0.76				1.01	2.08
O(11)	0.27	0.06	0.26	0.06	0.31						1.06	2.02
O(12)	0.26	0.07	0.22	0.15	0.33					1.06		2.09
O(13)	0.23	0.08	0.22	0.11	0.33			1.12				2.09
O(14)	0.27	0.08	0.19	0.15	0.32				1.04			2.05
W = F^-	$0.14^{\times 2\rightarrow}$	$0.02^{\times 2\rightarrow}$	$0.12^{\times 2\rightarrow}$	$0.02^{\times 2\rightarrow}$	$0.27^{\times 2\rightarrow}$							1.14
Σ	1.70		1.89		2.50	3.65	2.98	4.15	4.04	4.11	4.10	

*Bond valences in vu (valence units), bond-valence parameters from Gagné and Hawthorne (2015), except for F^- which are from Brese and O'Keefe (1991).

means that F^- cannot be replaced by $(OH)^-$ where the *A*, *B* and *M* sites are fully occupied as there is no room for the H^+ ion: it would be far too close to one or more of the surrounding cations. If there were vacancies at the locally associated *A*, *B* and/or *M* sites, would there be space for the H^+ ion involved in replacement of F^- by $(OH)^-$? Local association of a vacancy with an $(OH)^-$ group would still result in the H^+ ion being ~2.85 Å from an A, B or M cation; this distance is well within the coordination polyhedra of the A and B cations and hence is an arrangement that cannot occur. This argument accounts for the lack of significant substitution of F^- by $(OH)^-$ in the hyalotekite-group minerals.

The itsiite structure

The crystal structure of itsiite was solved by Kampf *et al*. (2014). The structure is topologically very similar to that of hyalotekite except that it is tetragonal (Table 1) with $T(1) \equiv T(2)$ and $F = \square$. To make itsiite easily comparable to the triclinic minerals of the hyalotekite group, we may write the formula of itsiite with $Z = 1$ as $Ba_4Ca_2[Si_8B_4O_{28}]\square$. In the structure of itsiite, the *T* tetrahedra form a four-membered ring where the *T* tetrahedra are equivalent, conforming to tetragonal symmetry. In the structure of the hyalotekite-group minerals, where more than one type of T cation is present (in those minerals currently approved), the tetragonal symmetry of the four-membered ring of *T* tetrahedra is broken by ordering of the T cations into different tetrahedra, reducing the symmetry to triclinic. Moreover, the *F* site, occupied by F^- in the known hyalotekite-group minerals, is vacant in itsiite.

A general formula

It is desirable to write a general formula for these minerals in terms of letters (in Roman font) that correspond reasonably with the site nomenclature of the hyalotekite structure. The *A* site of the structure is split into two sites, *A*(1) and *A*(2), with a separation sufficiently small that both sites cannot be occupied at the local scale; the *B* site shows the same behaviour. Thus in writing a general formula, we will ignore the splitting of these sites and consider just the *A* and *B* sites:

$$A_2B_2M_2[Si_8T_4O_{28}]F$$

where

$$A = Ba^{2+}, Pb^{2+}, K^+;$$
$$B = Ba^{2+}, Pb^{2+}, K^+;$$
$$M = Ca^{2+}, Y^{3+}, REE^{3+};$$
$$T = Si^{4+}, B^{3+}, Be^{2+}.$$
$$F = F^-, \square$$

Observed chemical compositions

There are currently three minerals with the (triclinic) hyalotekite-type structure and one with tetragonal symmetry and the same bond-topology (Table 1). The composition of kapitsaite-(Y) is written as $Ba_4Y_2[Si_8B_2B_2O_{28}]F$ in the current IMA list of minerals (Pasero *et al*., 2017), but this composition is not possible as it has a net charge of + 1. The only way that the structure can compensate for this charge is to replace one B^{3+} by one Be^{2+}. However, Pautov *et al*. (2000) did not report any Be^{2+} and the reported values for Si^{4+} and B^{3+} are not in accord with the presence of significant Be^{2+}; moreover, Y^{3+} is reported as 1.00 apfu with $Ca^{2+} =$ 0.78 apfu plus minor REE^{3+} and Na^+. The end-member formula of kapitsaite-(Y) should be written as neutral $Ba_4(YCa)[Si_8B_2B_2O_{28}]F$. The difference between khvorovite and hyalotekite is the dominant occupancy of the *A* and *B* sites by Pb^{2+} and Ba^{2+}, respectively. Previous chemical data for these minerals show a restricted variation in Pb^{2+}:Ba^{2+} ratio with most of the data lying within the field of hyalotekite. However, analysis of these minerals from Darai-Pioz shows complete solid solution between khvorovite and hyalotekite from Ba^{2+}-free to virtually Pb^{2+}-free compositions (Fig. 2). Where Ba^{2+} is the dominant cation, the K^+ content of the *A* sites is ~0.2 apfu. Where Pb^{2+} is the dominant cation, the K^+ content of the *A* sites increases linearly from ~0.2 apfu at $Pb^{2+} + K^+ = 2.0$ to ~0.9 apfu at $Pb^{2+} + K^+ = 4$ apfu. Kapitsaite-(Y) differs from hyalotekite in the ideal occurrence of equal amounts of Ca^{2+} and Y^{3+} at the *M* site (Pautov *et al*., 2000; Sokolova *et al*., 2000). The extensive solid-solution between khvorovite and hyalotekite at the Darai-Pioz locality suggests that a Pb^{2+}-analogue of kapitsaite-(Y) may be possible. For the chemical data currently available, there is no sign of any correlation between K^+ and Y^{3+} contents in these minerals.

Lindström (1887) reported significant Be^{2+} in hyalotekite from Långban, Värmland, Sweden, and Grew *et al*. (1994) showed that hyalotekite from the

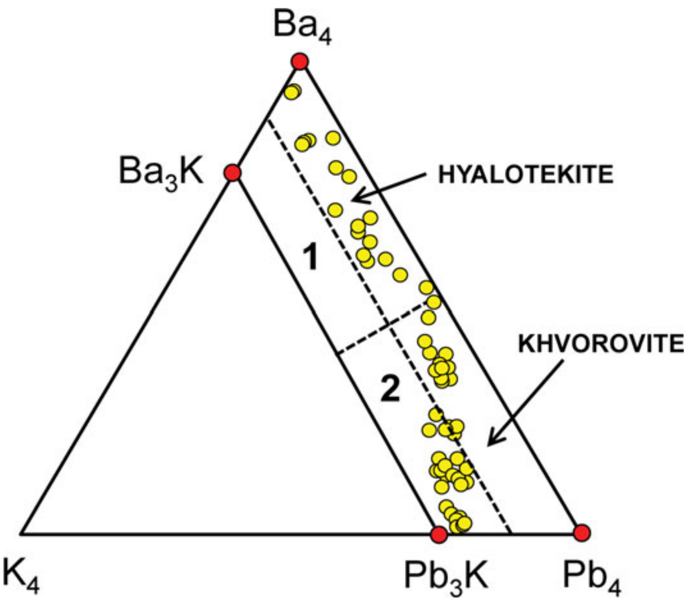

FIG. 2. Compositions of hyalotekite and khvorovite with the compositional fields of hyalotekite and khvorovite; end-member compositions are shown by red circles. The compositional field 1 defined by end-member A and B cations Ba_3K is empty, whereas compositional field 2 defined by end-member A and B cations Pb_3K contains analysed compositions. Data from Pautov *et al.* (2015).

Darai-Pioz alkaline massif, Tajikistan, also contains significant Be^{2+}. Thus we consider Be^{2+} as a significant constituent of the hyalotekite-group minerals.

Site occupancies

The tetrahedra of the framework are occupied by dominant cations Si^{4+} and B^{3+}. The < *Si*–O > distances reported by Sokolova *et al.* (2000) for kapitsaite-(Y), <Si–O> = 1.617 Å, and by Pautov *et al.* (2015) for khvorovite, <Si–O> = 1.617 Å, indicate that the *Si* sites are occupied only by Si^{4+} and that there is negligible substitution of B^{3+} at the *Si* sites. The < *T*(1)–O > distances are 1.480 and 1.478 Å in these two minerals, the same within one standard deviation as the grand < B^{3+}–O > distance of 1.476 Å reported for borate minerals by Hawthorne *et al.* (1996), indicating that the *T*(1) site is fully occupied by B^{3+} in kapitsaite-(Y) and khvorovite. However, we will show later that Be^{2+} must substitute for B^{3+} at the *T*(1) site in Be-bearing hyalotekite, and hence we allow for the substitution of Be^{2+} at the *T*(1) site in these minerals. Thus we will consider the $\{Si_8O_{28}F\}$ part of the structure as invariant and consider variable occupancies at the *A*, *B*, *M* and *T* sites as indicated by the general formula given above. Any future crystallographical data that indicates occupancy of the *Si* sites by cations other than Si^{4+} will require expansion of the present range of chemical formulae.

Enumeration of possible end-member compositions

The coordinations of the *A* and *B* sites are very similar and the site populations can only be determined by site-scattering refinement (Hawthorne *et al.*, 1995) combined with chemical analysis. Thus we have two possibilities in terms of defining possible end-member compositions: (1) we may amalgamate the *A* and *B* sites and produce a scheme that works for chemical analyses; (2) we may treat the *A* and *B* sites as distinct and produce a scheme that requires crystal-structure refinement for some compositions. It is trivial to derive the formulae for possibility (2) from those of possibility (1), and we will leave possibility (2) until it is shown to be of practical use,

The aggregate charge of the $\{Si_8O_{28}F\}$ part of the structure is 25^- and hence the aggregate charge of the cations occupying the ($A+B$), M and T sites is 25^+. Table 3 shows all end-member compositions conformable with the hyalotekite structure and having this aggregate charge. Of course, the end-member compositions of hyalotekite, khvorovite and kapitsaite-(Y) are represented here. However, there are many more possible end-member compositions, indicating the possibilities for new mineral species within this group.

Table 4 shows all end-member compositions conformable with tetragonal symmetry and with the F site as either vacant or occupied by F^-. Strict adherence to tetragonal symmetry requires that $T = B_4$ or Si_4. Composition 2 is itsiite (Table 1), and compositions 4–6 may be derived by inserting F^- at the F site; however, it is not clear if these compositions are possible with tetragonal symmetry, as $M=$ CaY and it is not clear whether Ca–Y will show long-range disorder or Ca–Y ordering will break the tetragonal symmetry. Note that compositions 4 and 5 in Table 4 are the same as compositions 5 and 6 in Table 3; only discovery of these compositions as minerals will reveal their symmetry.

Application to published compositions of hyalotekite-group minerals

The utility of this approach is immediately seen from inspection of Fig. 2 (modified from Pautov *et al.*, 2015). End-member compositions 3 and 4 are also shown on Fig. 2, and it is apparent that the compositional fields in the original figure were not correct. They have been corrected in Fig. 2 with the addition of end-member compositions 3 and 4 (Table 3). It is now apparent that several of the compositions presented by Pautov *et al.* (2015) fall within the compositional field defined by the end-member $(Pb^{2+}_3K)Ca_2[Si_8B_2Si_2O_{28}]F$ and deserve description as a new mineral.

The composition of a Pb-analogue of kapitsaite-(Y) from Darai-Pioz was given by Agakhanov *et al.* (2015).

TABLE 3. End-member compositions where A and B are not considered distinct.

Site	$A+B$	M	$T(1)$	$T(2)$	Si	B_{tot}	Si_{tot}
1*	Pb^{2+}_4	Ca^{2+}_2	$B^{3+}Si^{4+}$	B^{3+}_2	Si^{4+}_8	B^{3+}_3	Si^{4+}_9
2*	Ba^{2+}_4	Ca^{2+}_2	$B^{3+}Si^{4+}$	B^{3+}_2	Si^{4+}_8	B^{3+}_3	Si^{4+}_9
3**	Pb_3K^+	Ca^{2+}_2	Si^{4+}_2	B^{3+}_2	Si^{4+}_8	B^{3+}_2	Si^{4+}_{10}
4	Ba_3K^+	Ca^{2+}_2	Si^{4+}_2	B^{3+}_2	Si^{4+}_8	B^{3+}_2	Si^{4+}_{10}
5**	Pb^{2+}_4	$Ca^{2+}Y^{3+}$	B^{3+}_2	B^{3+}_2	Si^{4+}_8	B^{3+}_4	Si^{4+}_8
6*	Ba^{2+}_4	$Ca^{2+}Y^{3+}$	B^{3+}_2	B^{3+}_2	Si^{4+}_8	B^{3+}_4	Si^{4+}_8
7	Pb_3K^+	Y^{3+}_2	B^{3+}_2	B^{3+}_2	Si^{4+}_8	B^{3+}_4	Si^{4+}_8
8	Ba_3K^+	Y^{3+}_2	B^{3+}_2	B^{3+}_2	Si^{4+}_8	B^{3+}_4	Si^{4+}_8
9	Pb^{2+}_4	Y^{3+}_2	$Be^{2+}B^{3+}$	B^{3+}_2	Si^{4+}_8	B^{3+}_3	Si^{4+}_8
10	Pb^{2+}_4	Y^{3+}_2	$Be^{2+}B^{3+}$	B^{3+}_2	Si^{4+}_8	B^{3+}_3	Si^{4+}_8
11	Ba^{2+}_4	Y^{3+}_2	$Be^{2+}_{1.5}Si^{4+}_{0.5}$	B^{3+}_2	Si^{4+}_8	B^{3+}_2	Si^{4+}_8
12	Pb^{2+}_4	Ca^{2+}_2	Si^{4+}_2	$Be^{2+}B^{3+}$	Si^{4+}_8	B^{3+}_1	Si^{4+}_{10}
13	Ba^{2+}_4	Ca^{2+}_2	Si^{4+}_2	$Be^{2+}B^{3+}$	Si^{4+}_8	B^{3+}_1	Si^{4+}_{10}
14	Pb^{2+}_4	Y^{3+}_2	B^{3+}_2	$Be^{2+}B^{3+}$	Si^{4+}_8	B^{3+}_3	Si^{4+}_8
15	Ba^{2+}_4	Y^{3+}_2	B^{3+}_2	$Be^{2+}B^{3+}$	Si^{4+}_8	B^{3+}_3	Si^{4+}_8
16	Pb^{2+}_4	$Ca^{2+}Y^{3+}$	Si^{4+}_2	Be^{2+}_2	Si^{4+}_8	B^{3+}_0	Si^{4+}_{10}
17	Ba^{2+}_4	$Ca^{2+}Y^{3+}$	Si^{4+}_2	Be^{2+}_2	Si^{4+}_8	B^{3+}_0	Si^{4+}_{10}
18	Pb^{2+}_4	Y^{3+}_2	$B^{3+}Si^{4+}$	Be^{2+}_2	Si^{4+}_8	B^{3+}_1	Si^{4+}_9
19	Ba^{2+}_4	Y^{3+}_2	$B^{3+}Si^{4+}$	Be^{2+}_2	Si^{4+}_8	B^{3+}_1	Si^{4+}_9

*Composition corresponding to a known mineral species; ** composition corresponding to a valid un-named mineral species.

TABLE 4. End–member compositions derived from itsiite.

Site(s)	*A* + *B*	*M*	*T*	B$_{tot}$	Si$_{tot}$	F
1	Pb$_4^{2+}$	Ca$_2^{2+}$	B$_4^{3+}$	B$_4^{3+}$	Si$_8^{4+}$	$\square$
2*	Ba$_4^{2+}$	Ca$_2^{2+}$	B$_4^{3+}$	B$_4^{3+}$	Si$_8^{4+}$	$\square$
3	K$_4^{+}$	Ca$_2^{2+}$	B$_4^{3+}$	B$_0^{3+}$	Si$_8^{4+}$	$\square$
4	Pb$_4^{2+}$	Ca^{2+}Y^{3+}	B$_4^{3+}$	B$_4^{3+}$	Si$_8^{4+}$	F$^-$
5	Ba$_4^{2+}$	Ca^{2+} Y^{3+}	B$_4^{3+}$	B$_4^{3+}$	Si$_8^{4+}$	F$^-$
6	K$_4^{+}$	Ca^{2+} Y^{3+}	Si$_4^{4+}$	B$_0^{3+}$	Si$_8^{4+}$	F$^-$

*Composition corresponding to a known mineral species.

Christy *et al.* (1998) list ten chemical analyses for hyalotekite with B and Be analyses taken from Grew *et al.* (1994). These data were plotted by Hawthorne and Huminicki (2002) and again here in Fig. 3, which shows that the main substitution for incorporation of K in hyalotekite is K + Si → Ba + B. The one analysis plotting in the field Ba$_4$Ca$_2$[Si$_8$(BeB)Si$_2$O$_{28}$]F represents a new hyalotekite-type mineral

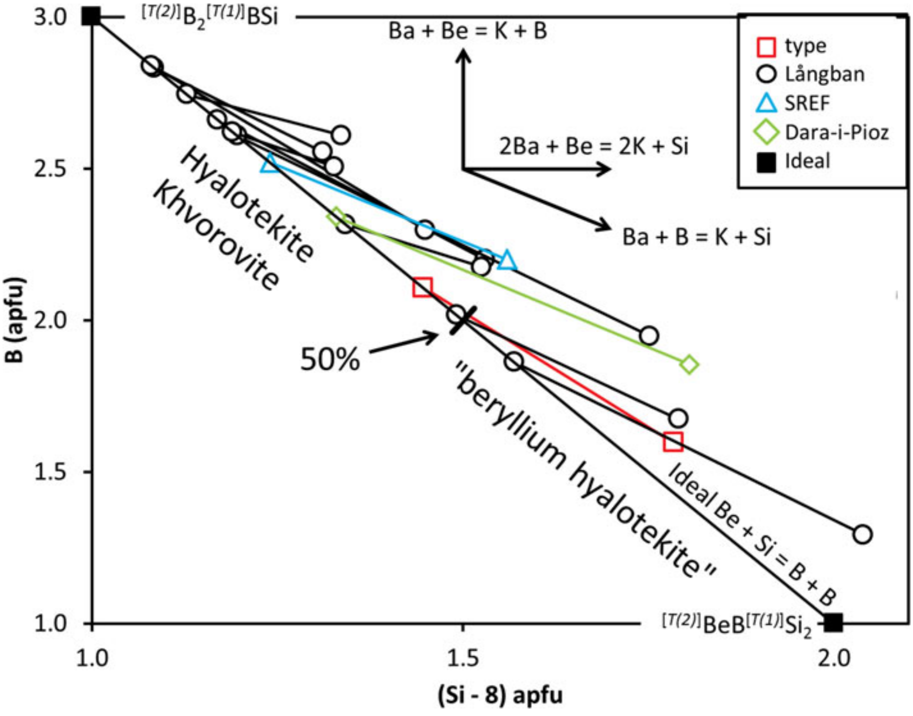

FIG. 3. Variation in B^{3+} as a function of (8 – Si^{4+}) in atoms per formula unit for hyalotekite composition following Hawthorne (2002, fig. 3). The ideal point $^{[T(1)]}$BeB$^{[T(1)]}$Si$_2$ corresponds to Ba$_4$Ca$_2$[Si$_8$(BBe)Si$_2$O$_{28}$]F, and the ideal point $^{[T(1)]}$B$_2^{[T(1)]}$SiB corresponds to Ba$_4$Ca$_2$[Si$_8$B$_2$(SiB)O$_{28}$]F. Each sample is represented by two points, one is the actual measured B and Si – 8 contents, the second is plotted on the join Be + Si = B + B and is calculated as 3 – 2*Be (*y* axis) *vs.* 1 + Be (*x* axis) in formula units. The line joining the two points gives the change in B and Si contents due to the substitution of Ba by K. Vectors give the three possibilities for this substitution (Hawthorne, 2002). SREF denotes a composition determined by site-scattering refinement. The field marked 'beryllium hyalotekite' indicates compositions in which the end-member component 13 (Table 3), Ba$_4$Ca$_2$[Si$_8$(BBe)Si$_2$O$_{28}$]F, is dominant: one analysis plots in this field: sample 114716, spot 2, from Långban. Sources of data: Grew *et al.* (1994) and Christy *et al.* (1998).

with essential Be^{2+}, that is, in which the end-member composition 13, $Ba_4Ca_2[Si_8(BeB)Si_2O_{28}]F$ (Table 3), is dominant.

Acknowledgements

We thank Fernando Cámara and Tony Kampf for their comments on this paper. The work was funded by a Discovery Grant from the Natural Sciences and Engineering Research Council of Canada.

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