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Crystal structure of cappelenite, $Ba(Y,RE)_6[Si_3B_6O_{24}]F_2$: a silicoborate sheet structure

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Abstract

Cappelenite, $Ba(Y,RE)_6[Si_3B_6O_{24}]F_2$, is based on a $^2_\infty[Si_3B_6O_{24}]$ tetrahedral corner-sharing sheet consisting of $[B_6O_{18}]$ six-membered and $[Si_3B_6O_{27}]$ nine-membered rings. The nine-membered rings are isomorphic to the insular $[Si_3Si_6O_{27}]$ rings in eudialyte. It is trigonal, a = 10.67(2), c = 4.680(2)Å, Z = 1, space group $P3$ with pronounced $P6mm$ symmetry through the *Zellengleich* relation $P3 \rightarrow P3ml \rightarrow P6mm$. R = 0.063 for 1450 independent reflections. The structure also is based on the $\{(6 \cdot 4 \cdot 3 \cdot 4)^4\}$ semi-regular net when the Y atoms are joined together in a plane parallel to {001} and may occur in other structures such as melanocerite, caryocerite, tritomite, *etc.* $[BaO_{12}]$ defines an hexagonal antiprism; $[YO_7F]$, square antiprisms; $[SiO_4]$ and $[BO_4]$, tetrahedra. The (Y,RE):F = 3:1 ratio appears to be characteristic for these lanthanide silicate compounds. Mean distances are $^{[12]}$Ba–O = 2.96, $^{[8]}$Y(1)–O = 2.38, $^{[8]}$Y(2)–O = 2.43, $^{[4]}$B(1)–O = 1.48, $^{[4]}$B(2)–O = 1.47 and $^{[4]}$Si–O = 1.64Å. The fluoride distances are 3F(1)–Y(1) = 2.38 and 3F(2)–Y(2) = 2.34Å.

Introduction

Cappelenite was named by the famous mineralogist–petrologist W. C. Brøgger (1885) honoring its discoverer, Mr. D. Cappelen of Holden, Norway. Only two specimens were found by Mr. Cappelen on the eastern side of the island Lille-Arø, a part of the nepheline syenites and pegmatitic syenitic veins in the mineralogically complex and classic Langesundfjord of Southern Norway. Brøgger (1890), in a definitive study, described the mineralogy of this region, which included over seventy species. Of these, over half were exotic titano- and zirconosilicates, beryllosilicates, borosilicates of alkalies, lanthanides and actinides, the last-mentioned usually occurring in a metamict state and amorphous to X-radiation. To restore crystallinity, such phases are usually heated, but it is not clear in powder diffraction studies whether reconstituted material is in fact representative of the original species, or is a product of recrystallization and/or decomposition of the parent structure. Therefore, Brøgger and coworkers afford a valuable service to our science through careful goniometric study and detailed chemical analyses.

Brøgger reported two specimens of this curious mineral, one a free crystal 2 cm in length and 1.5 cm in width, and a hand specimen displaying a broken crystal. Our interest in crystal-chemical systematics of the lanthanide silicates and borosilicates such as cerite, törnebohmite, steenstrupine, *etc.*, led to cappelenite, which has an unusual composition. Brøgger (1890) suggested $R^{3+}BO_3 \cdot R^{2+}SiO_3$ where R^{3+} = Y, La, Nd and R^{2+} = **Ba**, Ca, Na_2, K_2. Strunz (1970) proposed (Ba, *etc.*) $(Y, etc.)_2(B_2O_5)(SiO_4)$. Povarennykh (1972) offered $BaY_2(BSiO_5)(BO_4)$. More recently, Ramdohr and Strunz (1978) suggested $BaY_6B_6Si_3O_{25}$. Our crystal structure analysis admits the proposed composition $Ba(Y,RE)_6[Si_3B_6O_{24}]F_2$.

Experimental details

Fragments of the type material (collected by D. Cappelen, 1879) were kindly provided by Dr. Gunnar Raade of the Mineralogical-Geological Museum, University of Oslo. Small clear pale yellowish chips failed to provide any single crystal diffraction pattern and a metamict state was assumed. We were encouraged by Pabst (1961) who obtained excellent single crystal photographs of davidite through thermal reconstitution of previous metamict material. He reconstituted grains at temperatures between 1150°–1375°C. Lima de Faria (1956) noted that once reconstitution took place, the duration of heat treatment did not lead to further changes—a conclusion which Pabst also made.

For cappelenite, we were in essentially uncharted

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territory. Too high a temperature would lead to reconstructive recrystallization, decomposition, partial volatilization, *etc*. Too low a temperature would not promote any reconstitution. Since cappelenite appeared to be a silico-borate, the strategy was to start at some high temperature and proceed to successively lower temperatures for successive grains until satisfactory conditions were reached. A small fragment (*ca*. 0.1 mm) was placed in a quartz tube and heated in a small open air furnace at 1000°C for one week. The tube was then cooled and the grain microscopically inspected. It was cloudy and turbid, of a bile-green color. A single crystal photograph indicated recrystallization as only a powder pattern was obtained. The same phenomenon occurred at T = 900°C and 800°C, but at 700°C a faint but satisfactory single crystal photograph was obtained. Therefore, a clear grain of superior quality was heated for two weeks at 725°C. The reconstituted crystal provided superior single crystal X-ray photographs with Mo*Kα* radiation and Buerger precession camera. This was the same crystal used throughout the ensuing study.

Initial precession photographs of (*hk*0), (*h*0*l*) and (*hk*1) suggested condensed symbols *P*6/***. Since a complete data set was collected on a PICKER automated diffractometer, it became obvious that the equivalent reflections were related by lower symmetry. In fact, the ultimate structure refinement was performed in the group *P*3, in a direct group–subgroup relationship according to the *Zellengleich* genealogy *P*6/*mmm* → *P*6*mm* → *P*3*m*1 → *P*3.

One fragment measuring 0.33 mm ($\|a_1$) × 0.15 mm ($\|a_2$) × 0.12 mm ($\|c$) which was reconstituted at 725°C, was transferred to a PICKER automated diffractometer, using graphite monochromator and Mo*Kα* radiation (40 kV, 20 mA, $\lambda = 0.70926$Å). Prior to complete data collection, the cell parameters were refined, which yielded a = 10.67(2), c = 4.680(2)Å. The eventual success of the structure refinement suggested the space group *P*3 (pseudo *P*3*m*1). With scan speed 4° min^{-1}, base scan width of 2°, reflections to $2\theta = 70°$ ($\sin\theta/\lambda = 0.81$) were collected. Background counting times were 10 sec on each side of the peak. A total of 3606 reflections was collected ranging from $h = -14$ to $+16$, $k = -16$ to $+16$, $l = 0$ to $+7$. With linear absorption coefficient, $\mu \sim 212.1$ cm^{-1}, absorption correction was initiated using the AGNOST program. For the remainder of this study, the AGNOST program and the SHELX-76 program were run on the DEC VAX 11/780 computer facility at The University of Chicago. Symmetry equivalent reflections were then averaged according to eventual space group *P*3, yielding 1450 independent $|Fo|$.

Solution and refinement of the structure

The three-dimensional Patterson synthesis $P(uvw)$ led to eventual solution of the structure. Successive Fourier electron density maps admitted proper selection of the lighter atoms. Initially, Y was located in what appeared to be space group *P*6*mm*. Portions of the silicoborate sheet were identified and several positions were calculated according to earlier experience with the steenstrupine structure (Moore and Shen, 1983). The problem was not simple. Initially we assumed a $[B_6O_{18}]$ ring of {*C*3*i*} point symmetry, much like the $[Si_6O_{18}]$ ring in steenstrupine. At that stage we believed we had located the $[SiO_4]$ tetrahedra at (½ 0 0), (0 ½ 0), (½ ½ 0). Successive refinements did not converge below R = 0.22. It was then noted that the electron density about Y was severely distorted. Accordingly, the structure was refined in *P*3*m*1 but improvement was marginal. Finally *P*3 was selected, Y being split into two pseudosymmetric Y(1) and Y(2). At this stage, R = 0.16. Extra residues about Si forced us to

Table 1. Cappelenite: atomic coordinate parameters.†

Atom	K	x	y	z
Ba	1.00	0.0000	0.0000	0.0000
Y(1)	1.225(6)	0.2155(2)	0.4311(2)	0.9401(6)
Y(2)	1.160(6)	0.4320(2)	0.2161(2)	0.9722(9)
Si	1.00	0.0088(7)	0.5049(7)	0.4100(14)
B(1)	1.00	0.255(2)	0.255(2)	0.474(4)
B(2)	1.00	0.003(3)	0.254(2)	0.475(4)
O(1)	1.00	0.371(2)	0.387(2)	0.630(3)
O(2)	1.00	0.018(2)	0.387(2)	0.631(3)
O(3)	1.00	0.572(2)	0.428(1)	0.236(3)
O(4)	1.00	0.426(2)	0.573(2)	0.197(3)
O(5)	1.00	0.281(2)	0.140(2)	0.600(3)
O(6)	1.00	0.112(2)	0.227(2)	0.619(3)
O(7)	1.00	0.260(1)	0.262(1)	0.186(3)
O(8)	1.00	0.001(2)	0.265(2)	0.188(3)
F(1)	1.00	0.3333	0.6667	0.735(4)
F(2)	1.00	0.6667	0.3333	0.783(4)

†Estimated standard errors refer to the last digit. The site population parameter was varied only for Y(1) and Y(2).

Table 1a. Cappelenite: anisotropic thermal vibration parameters (×10^4).†

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ba	167(5)	$= U_{11}$	194(14)	0	0	$= \frac{1}{2} U_{11}$
*Y(1)	1(6)	39(6)	107(6)	-21(5)	1(4)	14(6)
Y(2)	40(8)	88(9)	173(7)	-49(7)	-56(7)	11(7)
Si	116(21)	74(19)	217(27)	31(20)	17(21)	45(17)
*O(1)	149(43)	234(46)	22(39)	20(38)	62(36)	78(38)
O(2)	316(50)	230(47)	156(47)	44(42)	-93(44)	156(41)
O(3)	179(44)	18(37)	129(44)	-26(35)	- 3(39)	21(34)
O(4)	70(39)	106(41)	181(45)	-39(39)	-37(37)	25(34)
O(5)	125(41)	190(44)	209(47)	20(41)	39(40)	115(36)
O(6)	229(46)	244(47)	288(51)	25(45)	-35(44)	190(39)
*O(7)	1(36)	79(40)	247(46)	-73(38)	-38(36)	9(31)
O(8)	109(42)	167(44)	192(46)	22(40)	88(39)	69(36)
*B(1)	128(45)	1(38)	245(51)	2(40)	32(43)	175(34)
*B(2)	320(58)	1(46)	151(52)	-70(46)	-89(52)	-37(48)
F(1)	Beq = 1.14(29) Å^2					
F(2)	Beq = 0.94(28) Å^2					

†Coefficients in the expression $\exp-[U_{11}h^2 + U_{22}k^2 + U_{33}\ell^2 + 2U_{23}k\ell + 2U_{13}h\ell + 2U_{12}hk]$. Estimated standard errors refer to the last digit.

*Atoms with non-positive definite parameters. It is not known if this is due to pseudosymmetry or errors in absorption correction.

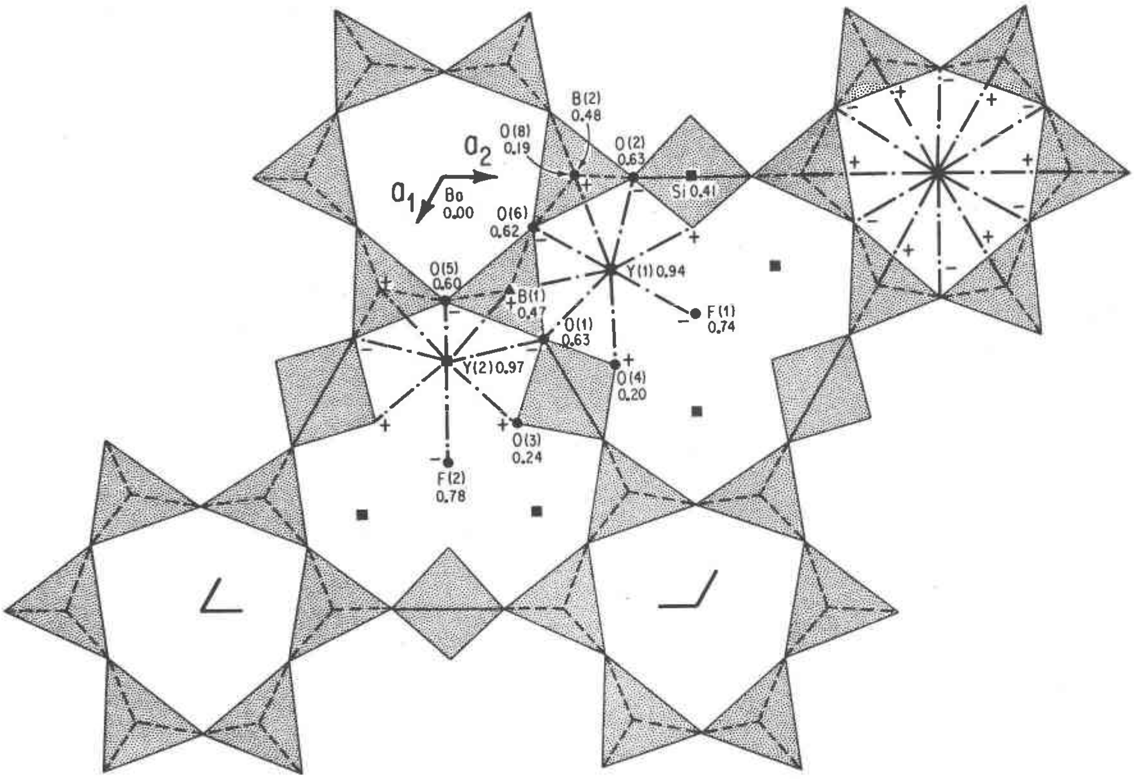

Fig. 1. Projection down *c* of the $[Si_3B_6O_{24}]$ sheet in cappelenite. The tetrahedral sheet is stippled and the Y–O, F and Ba–O bonds are drawn as spokes. Atom heights in the asymmetric unit are given as fractional coordinates in *z*. Anions which are relatively above (+) or below (−) the coordinated large cation are noted accordingly. The symmetry is approximately *P6mm*.

invert the tetrahedral orientation, leading to a $[B_6O_{18}]$ ring of $\{C3\}$ symmetry. Convergence was then rapid, and led to $R = 0.063$ for all 1450 unique reflections where

$$R = \frac{\Sigma||F_o| - |F_c||}{\Sigma|F_o|}.$$

Scattering curves for Y^{3+}, Si^{4+}, B^{3+} and $F^- = O^{2-} = O^{0+}$ were obtained from Ibers and Hamilton (1974). Anomalous dispersion correction, f″, was built into the SHELX-76 program.

We also refined the structure in *P*3*m*1, and in *P*3 but without absorption correction. For the former, $R = 0.12$ and for the latter, $R = 0.17$. This demonstrates that pseudosymmetry can present a problem in lanthanide oxysalt structures (compare wtih Voronkov and Pyatenko, 1967; for the stillwellite structure) and that absorption correction is of major importance: it is our experience that for lanthanide silicates, the correct lanthanide atom positions alone usually lead to $R \sim 0.25$.

Atomic coordinate parameters are presented in Table 1, thermal vibration parameters in Table 1a, structure factor tables in Table 2,[1] bond distances and angles in Table 3, chemical interpretation in Table 4 and electrostatic valence balances in Table 5.

Description of the structure

Cappelenite possesses an aesthetically pleasing structure. Its principle is based on a silicoborate sheet of composition $^{3}_{\infty}[Si_3B_6O_{24}]^{18-}$. The sheet can be dissected into $[B_6O_{18}]$rings of point symmetry approximating $\{C6\}$, and $[Si_3B_6O_{27}]$ of point symmetry $\{C3\}$. The hexagonal ring is one of thirteen admissible types based on apical oxygens (Moore, 1973). In cappelenite, all the apical oxygens point in one direction, which is *down* in Figure 1.

At first, the nonameric ring appeared unusual to us, but it is isomorphic to the $[Si_9O_{27}]$ ring in eudialyte, reported in a detailed study by Giuseppetti *et al.* (1971). In fact, their Figure 1 and our nonamer closely match about (⅔, ⅓), except for minor tiltings of the tetrahedra. Eudialyte is, to a first approximation,

$$Na_{12}Ca_6Fe^{2+}_3Zr^{4+}_{3.25}[Si_9O_{24}(OH)_3]_2[Si_3O_9]_2\ Cl;$$
$$R3m,\ a = 14.24,\ c = 30.08Å,\ Z = 3.$$

It is noted in eudialyte's structure that the *a*-translation of the compound should nearly match that of cappelenite by condensing the O(2) atoms together related by the mirror plane. They correspond to an edge of the $Zr(1)O_6$ octahedron. We conceive such a condensation by elim-

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[1] To receive a copy of Table 2, order Document AM-83-237 from the Business Office, Mineralogical Society of America, 2000 Florida Avenue, N.W., Washington, D.C. 20009. Please remit $5.00 in advance for the microfiche.

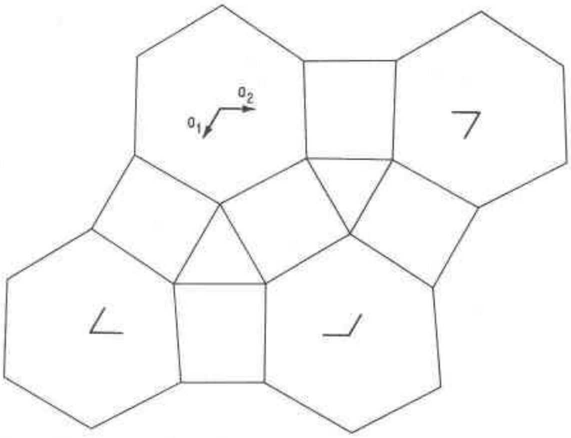

Fig. 2. Connecting the nearly coplanar Y atoms projected down *c* leads to the $\{(6 \cdot 4 \cdot 3 \cdot 4)^4\}$ semi-regular net. Note the large Ba^{2+} resides in the hexagons, the $(SiO_4)^{4-}$ tetrahedra in the squares and the F^- anions in the triangles. This was drawn directly from the Y atomic coordinates.

inating the Zr(1) atom, the $[Si_3O_9]$ ring and fusing the O(2) oxygens together on the mirror plane. As a result, a tetrahedral sheet is created, based on the same 6-membered and 9-membered rings discussed in this paper, with composition ${}^{2}_{\infty}[Si_9O_{24}]^{12-}$. Fusion of O(2) allows us to metrically compare cappelenite and eudialyte. This calculation yields:

	cappelenite	"condensed" eudialyte
	$[Si_3B_6O_{24}]^{18-}$	$[Si_3Si_6O_{24}]^{12-}$
a	10.66Å	11.43Å

the only difference being a shrinkage for cappelenite owing to the smaller borate tetrahedron. We speculate that a "condensed" eudialyte may indeed exist, with probable trigonal or rhombohedral symmetry. Such a hypothetical compound would occur in nepheline syenites which display eudialyte and anticipated mimetic relationships may render the compound difficult to recognize as a possibly unique substance. A possible composition could be $Na_4Ca_2Zr[Si_9O_{24}]$. Other candidates may include the metamict trigonal minerals from the same region: melanocerite, caryocerite and tritomite.

A common thread is emerging among the yttrium and lanthanide-bearing silicates and borosilicates. The large lanthanide and alkaline earth cations are often distributed so that a rod description is appealing. Furthermore, connecting the projection points of the rods to each other often yields semi-regular nets which greatly ease in structure description. Thus, cerite, whitlockite and steenstrupine are based on the $\{(6 \cdot 3 \cdot 6 \cdot 3)^4\}$ Kagomé net, whereas fillowite and apatite are based on the $\{6^3\}$ hexagonal net. In cappelenite, the Y atoms lie nearly in a plane. Connecting them yields Figure 2, the $\{(6 \cdot 4 \cdot 3 \cdot 4)^4\}$ semi-regular net. Including the other structures, the very large cations, disordered anions; F^-, OH^- anions or octahedral face-sharing cations occur in the centers of the hexagons.

Cappelenite has large Ba^{2+} situated in the center of the hexagon at the origin of the cell, in an hexagonal antiprismatic coordination by oxygens. Another interesting pattern emerges. For cerite, $RE_9Fe^{3+}[SiO_4]_6[SiO_3OH](OH)_3$; steenstrupine, $Na_{14}RE_6Mn_2Fe^{3+}{}_2(Zr,Th)(OH)_2[PO_3OH][PO_4]_6[Si_6O_{18}]_2 \cdot 3H_2O$ and britholite, $Ca_2RE_3(OH)(SiO_4)_3$, three large lanthanides coordinate to one $(OH)^-$ or F^- ligand situated on the rod at (0 0 *z*). This phenomenon is so frequently encountered among the lanthanide minerals that a polyhedral expansion principle seems to be operating. This is best illustrated for the pseudo-isomorphic pair whitlockite-cerite, where $Ca_9\phi_n$–$RE_9\phi_n(OH)_3$ occurs, ϕ representing any other coordinating ligands.

Cappelenite displays the same phenomenon. Three Y coordinate to one F^- ligand at (⅔,⅓), (⅓,⅔). Thus, the coordination polyhedron expands from YO_7 to YO_7F. The F(1)–O(4) and F(2)–O(3) edges are shared by pairs of Y(1) and Y(2) atoms. In many respects the structure can be conceived as the linkage of two layers, the $[B_3Si_6]$ cation layer at $z \sim \frac{1}{2}$ and the $[BaY_6]$ layer $z \sim 0$ through

Table 3. Cappelenite: bond distances and angles.†

Ba		
3 Ba-O(6)	2.75	
3 -O(7)	2.92	
3 -O(8)	2.95	
3 -O(5)	3.20	
average	2.96 Å	

Si		angle (deg.)
Si-O(3)	1.62	
-O(4)	1.62	
-O(1)	1.65	
-O(2)	1.66	
average	1.64	
O(1)-O(2)	2.58	102.7
O(1)-O(3)	2.69	110.4
O(1)-O(4)	2.69	110.9
O(2)-O(4)	2.69	109.7
O(3)-O(4)	2.69	112.1
O(2)-O(3)	2.70	110.7
average	2.67	109.4

F		
3 F(1)-Y(1)	2.38	
3 F(2)-Y(2)	2.34	
average	2.36	

B(1)		angle (deg.)
B(1)-O(7)	1.35	
-O(5)	1.50	
-O(1)	1.52	
-O(6)	1.55	
average	1.48	
O(1)-O(5)	2.31	99.9
O(5)-O(6)	2.39	103.7
O(5)-O(7)	2.40	114.6
O(1)-O(6)	2.41	103.6
O(1)-O(7)	2.43	115.5
O(6)-O(7)	2.48	117.3
average	2.40	109.1

B(2)		
B(2)-O(8)	1.35	
-O(6)	1.50	
-O(5)	1.51	
-O(2)	1.53	
average	1.47	
O(2)-O(5)	2.32	99.5
O(2)-O(6)	2.38	103.7
O(5)-O(6)	2.38	104.5
O(5)-O(8)	2.40	114.0
O(2)-O(8)	2.41	113.1
O(6)-O(8)	2.48	120.4
average	2.40	109.2

Y(1)	
Y(1)-O(4)	2.32
-O(4)′	2.32
-O(7)	2.38
-O(8)	2.38
-F(1)	2.38
-O(2)	2.40
-O(6)	2.41
-O(1)	2.42
average	2.38

Y(2)	
Y(2)-O(5)	2.23
-O(3)	2.34
-O(3)	2.34
-O(7)	2.34
-O(8)	2.34
-F(2)	2.34
-O(1)	2.73
-O(2)	2.75
average	2.43

†Estimated standard errors are Ba-, Y-, Si-O ± 0.02; B-O ± 0.03; Y-F ± 0.01; and O-O′ ± 0.03 Å. The angles are ± 1.4°.

Table 4. Cappelenite: chemical analysis.

	1	2	3	4
K_2O	0.20	---	0.05	--
Na_2O	0.25	---	0.10	--
BaO	8.02	12.35	0.64	1
CaO	0.67	---	0.15	--
La_2O_3	2.97	---	0.22	--
Y_2O_3	52.62	54.55	5.74	6
B_2O_3	[17.16]	16.82	6.07	6
ThO_2	0.80	---	0.04	--
CeO_2	1.29	---	0.09	--
SiO_2	14.21	14.51	2.91	3
F	---	3.06		[2]
Ignition	1.81	---		--
Total	100.00	101.29 1.29	16.01	16
− ½O = F	---	100.00		

[1] P. T. Cleve analysis in Brøgger (1890). The B_2O_3 content was determined by difference. F was sought but not found.

[2] Theoretical weight percent for $BaY_6[Si_3B_6O_{24}]F_2$.

[3] Cation content based on 50 electrons.

[4] Theoretical content for $BaY_6[Si_3B_6O_{24}]F_2$.

the interleaving anions at $z \sim 1/4, 3/4$. Alternatively, it can be conceived as the fusion of the two principal sheets, $[Si_3B_6O_{24}]^{18-}$ and $[BaY_6O_{24}F_2]^{30-}$ at all the oxide anions. In the latter, (BaO_{12}) hexagonal antiprisms and (YO_7F) square antiprisms comprise the polyhedral units.

Crystal chemistry

Bond distances and tetrahedral angles are given in Table 3. The calculated bond distances from Shannon and Prewitt (1969), with correction for mean anion coordination by cations, stand in fairly good agreement with the averages reported herein. The observed averages followed by the calculated distances in parentheses are: $^{[12]}$Ba–O = 2.96(2.98), $^{[8]}$Y(1)–O = 2.38(2.38), $^{[8]}$Y(2)–O = 2.43(2.38), $^{[4]}$Si–O = 1.64(1.63), $^{[4]}$B(1)–O = 1.48(1.50), $^{[4]}$B(2)–O = 1.47(1.50)Å.

Table 5. Cappelenite: electrostatic valence balance of cations and anions.†

	Coordinating Cations						
	Ba	Y(1)	Y(2)	Si	B(1)	B(2)	Δp_o
ζ →	$^2/_{12}$	$^3/_8$	$^3/_8$	$^4/_4$	$^3/_4$	$^3/_4$	
Anions							
O(1)	-----	$\underline{+0.04}$	$\underline{+0.30}$	$\underline{+0.01}$	$\underline{+0.04}$	-----	+0.50
O(2)	-----	$\underline{+0.02}$	$\underline{+0.32}$	$\underline{+0.02}$	-----	$\underline{+0.06}$	+0.50
O(3)	-----	-----	$\underline{-0.09\ (\times 2)}$	$\underline{-0.02}$	-----	-----	-0.25
O(4)	-----	$\underline{-0.06\ (\times 2)}$	-----	$\underline{-0.02}$	-----	-----	-0.25
O(5)	$\underline{+0.24}$	-----	-0.20	-----	$\underline{+0.02}$	$\underline{+0.04}$	+0.04
O(6)	-0.21	$\underline{+0.03}$	-----	-----	$\underline{+0.07}$	$\underline{+0.03}$	+0.04
O(7)	$\underline{-0.04}$	$\underline{+0.00}$	$\underline{-0.09}$	-----	$\underline{-0.13}$	-----	-0.33
O(8)	$\underline{-0.01}$	$\underline{+0.00}$	$\underline{-0.09}$	-----	-----	$\underline{-0.12}$	-0.33
F(1)	-----	+0.00	-----	-----	-----	-----	+0.12
F(2)	-----	-----	-0.09	-----	-----	-----	+0.12

†A bond length deviation refers to the polyhedral average subtracted from the individual bond distance. The Δp_o = deviations of electrostatic bond strength sum from neutrality (p_o = 2.00 e.s.u. for O^{2-} and 1.00 e.s.u. for F^-). Bond length deviations which conform to Δp_o are underlined.

We saw no need to re-analyze cappelenite since but little material exists and since the great range of elements present would pose serious problems for even modern spectroscopic techniques. Consequently, the analysis of P. T. Cleve (In Brøgger, 1890) is presented in Table 4 along with calculations for end-member $BaY_6[Si_3B_6O_{24}]F_2$. Fluorine was reported to be sought but not found in the earlier study. Since we found extra electron density at (⅔, ⅓), (⅓, ⅔) and since this could be easily explained by F^- and/or OH^- anions we submitted a small grain to ARL electron microprobe analysis for fluorine. At present, this mode of analysis is semi-quantitative at best on our instrument. Although fluorine was detectable, no reliable content could be obtained. We suspect that the greater fraction of ignition reported in Brøgger (1890) may indeed be tightly bound fluorine. The presence of thoria is probably the source of the metamict state for the mineral.

We arranged the cations reported by Cleve according to decreasing effective ionic radii for 6-coordination and partitioned them into the respective structural sites. The result is: $(K_{0.05}Ba_{0.64}La^{3+}_{0.22}Na_{0.10})_{\Sigma=1.01}(Th^{4+}_{0.04}Ca_{0.15}Y_{5.74}Ce^{4+}_{0.09})_{\Sigma=6.02}Si_{2.91}B_{6.07}O_{24}F_2$, which is in satisfactory agreement with the end-member formula adopted in this study.

Finally, when a structure is known, it is often advantageous to perform a bond strength sum calculation of cations about anions. This is presented in Table 5. In general, agreement between individual bond distance deviations from polyhedral averages with deviations of electrostatic bond strength sum from neutrality is quite satisfactory: of 32 entries, 28 show agreement, or 88% of the total entries. The most pronounced deviations correspond to O(7) and O(8), each with $\Delta p_o = -0.33$ e.s.u. This extreme undersaturation may explain the unusually short $^{[4]}$B(1)–O and $^{[4]}$B(2)–O = 1.35Å distances, values which would be close to $^{[3]}$B–O ~ 1.40Å.

Another curious feature is the difference between the Y(1)–O = 2.38 and Y(2)–O = 2.43Å bond distance averages and the site population refinements, both of which indicate an average atomic number greater than Y^{3+}. This segregation between Y(1) and Y(2) may be the reason for superior refinement in *P*3 in the *Zellengleich* sequence *P6mm* → *P3m*1 → *P*3. Topologically, the cappelenite structure is *P6mm* and pure crystals of the end-member composition may indeed satisfy this space group.

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