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The crystal structure of sulfoborite, $Mg_3SO_4(B(OH)_4)_2(OH)F$

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Abstract

Sulfoborite, $Mg_3SO_4(B(OH)_4)_2(OH)F$, is orthorhombic, space group *Pnma* with $a = 10.132$, $b = 12.537$ and $c = 7.775$Å (all ±0.001Å). There are four formula units in the unit cell. The crystal structure has been solved using Sayre's equation. All atoms including hydrogens have been located and refined by least squares to an R-value of 0.044. The magnesium ions are of two types; $MgO_2F(OH)_3$ and $MgOF(OH)_4$. The two types of octahedra share an edge and/or corners among themselves. The sulphate tetrahedron shares corners with both types of octahedra and these three units form crude sheets centered about the mirror planes. The sheets are jointed by the boron tetrahedra into a three-dimensional structure. Three hydrogen atoms do not participate in hydrogen bonding, the remaining two form normal hydrogen bonds.

Introduction

The original descriptions of sulfoborite indicated a chemical formula of $Mg_6H_4(BO_3)_4SO_4{\cdot}7H_2O$ (Naupert and Wense, 1893) and orthorhombic symmetry with point group *mm*2 (Bücking, 1893). The mineral has been studied several times since 1893 and no agreement as to the chemical composition was evident. Lobanova (1968) proposed the formula $Mg_6B_4O_{10}(SO_4)_2{\cdot}9H_2O$ even though his published analysis indicated 4.7% fluorine and 0.34% chlorine. Braitsch (1961) suggested $Mg_6SO_4(BO_2OH)_4{\cdot}8H_2O$ as the formula and confirmed by single crystal X-ray diffraction the orthorhombic symmetry. He could not distinguish between the space groups *Pcmn* and $Pc2_1n$. Kondrat'eva (1964) analyzed several samples and confirmed the Lobanova formula. More recently, Ostrovskaya (1967) used infrared spectroscopy to demonstrate the presence of hydroxyl and the absence of water indicating that previous analyses had incorrectly equated OH to H_2O. In addition, it was concluded that the boron was tetrahedrally and not trigonally coordinated.

The major differences between these proposed formulae lie in the amounts of water of hydration, hydroxyl and hydrogen. At the time this work was begun, we were not aware of Ostrovskaya's paper and we felt that a crystal structure determination was the only way to resolve these questions. Since the mineral contains only light elements, it was hoped that the hydrogen atoms could be located and refined. The resulting structure would, in addition to resolving the question of the chemistry of sulfoborite, provide some interesting information about hydrogen bonding and the role of fluorine and hydroxyls in this structure. A preliminary report of the structure analysis was presented by Giese and Penna (1968). Ioryish *et al.* (1976) have published an independent structure determination which differs from that of Giese and Penna in being less accurate, in apparently misidentifying one of the anions and in not locating the hydrogen atoms. For these very important reasons, the structure is reported here.

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Experimental

A large, transparent crystal from Westeregeln, Germany was obtained from the Royal Ontario Museum (catalog #M6918). This was broken into a roughly equidimensional fragment 0.2 mm in diameter, mounted on a goniometer and examined with a General Electric XRD-5 equipped with a single crystal orienter. The initial study as well as data collection used Mo$K\alpha$ radiation and a scintillation counter. The crystal was found to be orthorhombic and the least-squares refined cell parameters are $a = 10.132$, $b = 12.537$, and $c = 7.775$Å (all ±0.001Å). The systematic extinctions are:

hkl	no conditions
$hk0$	$h = 2n$ present
$h0l$	no conditions
$0kl$	$l = 2n$ present
$h00$	$h = 2n$ present
$0k0$	no conditions
$00l$	$l = 2n$ present

The number of formula units was assumed to be four as reported by Braitsch (1961). The two possible space groups are *Pnma* and $Pn2_1a$. All X-ray reflections with 2θ less than 60° were measured using a stationary crystal–stationary counter technique and balanced filters. There were 1502 unique reflections within this sphere and only 14 were unobserved.

An empirical absorption correction was made by measuring the intensity of the (600) reflection with the single crystal orienter set at chi = 90°. The intensity of this reflection was measured as a function of the angular setting phi at intervals of 10°. These intensities were normalized and the resulting values were used to modify the observed intensities. The maximum correction was 8% indicating that absorption errors with Mo radiation were small. The raw intensities were corrected for Lorentz and polarization factors in the usual manner. The unscaled structure factors were converted to normalized structure factors by the method of Hauptman and Karle (1953). The distribution of the E's was found to be:

	Obs.	Exp. centric	Exp. acentric
average E^2	0.996	1.000	1.000
average E	0.806	0.798	0.886
average $\lvert E^2-1\rvert$	0.961	0.968	0.736
E > 1	0.308	0.32	0.37
E > 2	0.04	0.05	0.02
E > 3	0.002	0.003	0.0001

These values indicate that the true space group is *Pnma* and subsequent study has verified this.

Structure determination

The procedure was to use repetitively Sayre's equation (Sayre, 1952)

$$sE_H = s\sum_K E_H E_{H-K}$$

where s means "sign of". A computer program written by Long (1965) performed the calculations. It first assigned plus signs to three reflections, (452), (301) and (441) to fix an origin and then took four additional reflections (303), (4.13.2), (432) and (10.4.5) which were assigned plus or minus until all combinations had been tried, a total of 2^4. For each starting set of 7 reflections, all other signs were determined with Sayre's equation. The program goes through the list of E's (all E's greater than 1.5 were used) until no new signs are added or no changes in sign are made. For each set, a consistancy index is computed—

$$C = \frac{\left\langle \left| E_H \sum_K E_H E_{H-K} \right| \right\rangle}{\left\langle \left| E_H \right| \sum_K \left| E_H \right| \left| E_K \right| \right\rangle}$$

The correct set of signs usually has the least number of cycles required for convergence and the highest value of C. For sulfoborite, one set of starting signs yielded C = 0.90 (1.00 is the maximum) and the set converged in 6 cycles, the least number for all starting sets of signs.

A three-dimensional Fourier map was computed using the signed E values for this set. From the map, coordinates for 13 atoms were obtained. The initial *R* factor with these atoms treated as oxygen was 0.50 and in 3 cycles of least-squares refinement this decreased to 0.37. Thereafter, the procedure was to perform a few cycles of least-squares refinement and look at the difference electron density map for missing atoms. All the non-hydrogen atoms were located after going through this sequence twice. The isotropic thermal parameters and the electron density in the difference map at each atomic site indicated the essentially correct assignment of scattering factors for each atom. At this point there was no indication either from the refinement or previous chemical data that fluorine might be present in the structure. The isotropic thermal parameter refinement converged at $R = 0.077$.

Final refinement

The scattering factors of Cromer and Weber (1965) for neutral atoms were used for oxygen, boron and hydrogen while ionized atom scattering values were used for sulphur, magnesium and fluorine. The least-squares program was a modification of a block diagonal routine written by Ganzel, Sparks and Trueblood. Anisotropic thermal parameters for all non-hydrogen atoms, their positional parameters and an overall scale factor were then refined with convergence at $R = 0.057$. At this point, a difference electron density map showed the positions of 5 hydrogen atoms. In addition, the electron density at the site of one of the oxygen atoms was rather high and the hydrogen atom required by the local charge balance was not visible in the difference map. Both observations suggested that the site was occupied by a single monovalent anion rather than OH. These results follow closely the experience of Guy and Jeffrey (1966) in their study of the crystal structure of fluellite. Fluorine was a natural candidate in view of its similar scattering power compared to oxygen. Several further cycles of refinement, including fluorine, removed all major anomalies in the difference electron density map. The *R* factor dropped slightly but there was a great improvement in the standard deviations for the positional parameters of many atoms. It was only after the fluorine had been positively identified on the basis of the final refinement of the structure that the chemical analysis of Lobanova (1958) was found. The X-ray structure called for 5% fluorine and Lobanova had reported 5.04% fluorine + chlorine.

To avoid any possible bias in locating the hydrogen atoms, a structure model was not constructed until all candidate hydrogens had been located in difference electron density maps and subjected to isotropic least squares refinement. All the positional parameters for the hydrogens converged as did their isotropic thermal parameters. At this stage of the determination we still expected to find several water molecules but no more hydrogen atoms could be located and in fact there were only 5 peaks with values greater than twice the background. Only after computing interatomic distances and building a model of the structure was it clear that only hydroxyls were present. The resulting structure is in complete agreement with the infrared study of Ostrovskaya (1967).

Discussion

Table 1 lists the fractional coordinates for all atoms, Table 2 lists the anisotropic thermal parameters for all non-hydrogen atoms. Observed and calculated structure factors are listed in Table 3.[1] Bond distances are shown in Table 4 and Table 5 lists the hydrogen bonding distances and angles. One of the magnesium atoms, Mg(1), lies on a mirror plane, the other, Mg(2), is on a general position. Sulphur lies on the mirror plane and boron in a general position. The magnesium ions are octahedrally coordinated while both boron and sulphur are tetrahedrally coordinated. The Mg(1) octahedron shares two vertices with the Mg(2) octahedron, and two Mg(2) octahedra share the edge lying in the mirror plane (Figs. 1 and 2). The octahedra form an undulating chain in the *a*-axis direction. The shared edge between Mg(2) octahedra is formed by F and O(7) and has a relatively short length of 2.608Å compared with values between 2.805 and 3.134Å for other octahedral edges. This is to be expected from the close approach of the Mg(2) ions (3.106Å). The fluorine and oxygen are not distinguishable on the basis of the distances to the magnesium or to neighboring anions. In fact, the less accurate structure determination of Iorysh *et al.* (1976) could not, independent of chemical evidence, identify the presence of fluorine in the

Table 1. Positional parameters for the atoms in sulfoborite in fractions of the unit cell edge. The figures in parentheses are standard deviations.

Atom	x	y	z
B	0.3186(3)	0.5028(2)	0.0854(3)
Mg(1)	.1838(1)	1/4	.4849(1)
Mg(2)	.0687(1)	.6261(1)	.2504(1)
S	.4883(1)	1/4	.3901(1)
F	.4700(1)	3/4	.1468(2)
O(1)	.4939(2)	.6538(2)	.5019(2)
O(2)	.3538(2)	1/4	.3167(2)
O(3)	.0851(2)	1/4	.2479(3)
O(4)*	.1699(2)	.4091(1)	.4674(2)
O(5)*	.1800(2)	.4968(1)	.1532(2)
O(6)*	.1496(2)	.5965(1)	.4931(2)
O(7)*	.1985(1)	3/4	.1985(2)
O(8)*	.4081(2)	.5241(1)	.2297(2)
H(1)	.148(3)	.456(3)	.111(4)
H(2)	.175(3)	.426(3)	.375(5)
H(3)	.355(3)	.362(3)	.047(4)
H(4)	.395(4)	.494(3)	.298(4)
H(5)	.229(4)	3/4	.254(4)

* hydroxyl

Table 2. Thermal parameters (× 10^5 for the anisotropic parameters). The temperature factor is $\exp(-\{B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{13}hl + B_{23}kl\})$

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}	B_{iso}
S	174(11)	115(12)	238(15)	0	87(30)	0	
Mg(1)	190(15)	106(17)	305(22)	0	-26(15)	0	
Mg(2)	184(7)	133(4)	317(12)	0(10)	41(15)	42(14)	
B	157(21)	100(14)	184(36)	12(28)	64(45)	-36(36)	
F	179(25)	124(32)	424(39)	0	-160(32)	0	
O(1)	345(17)	160(10)	406(27)	-126(22)	257(34)	-161(21)	
O(2)	179(35)	305(40)	441(50)	0	-161(31)	0	
O(3)	319(35)	229(40)	426(52)	0	-472(40)	0	
O(4)	371(17)	103(10)	255(25)	-32(21)	-57(35)	-6(27)	
O(5)	136(14)	157(10)	374(27)	-45(20)	66(33)	-99(27)	
O(6)	302(16)	115(10)	344(27)	68(21)	-133(34)	-19(28)	
O(7)	131(31)	163(35)	244(45)	0	-61(37)	0	
O(8)	252(16)	197(10)	275(26)	-96(22)	-118(33)	74(29)	
H(1)							-0.32(64)
H(2)							0.61(82)
H(3)							-0.24(66)
H(4)							0.15(87)
H(5)							-1.40(70)

structure. Only the small discrepency of electron density in the difference map and the absence of a nearby hydrogen give direct X-ray evidence that fluorine is in the structure. In the same mirror plane, the sulphate tetrahedra join these chains, the connection going from an octahedron in the plane in one chain to the two edge-sharing octahedra in the chain above or below in the *c*-axis direction.

The magnesium and sulphate polyhedra form continuous sheets centered about the mirror planes at y = ¼ and ¾. The bonding between sheets is through the boron tetrahedra (Fig. 2). The edge sharing octahedra are tilted toward each other; the

Table 4. Interatomic distances for the polyhedra. The standard deviations are given in parentheses.

Octahedral Sites

Mg(1)	F	2.003(1)	O(4) --	F	2.817(1)
	O(2)	2.163(2)		O(2)	2.970(2)
	O(3)	2.097(2)		O(3)	2.762(2)
	O(4)	2.042(2)		O(7)	2.997(2)
	O(7)	2.045(2)	O(3) --	F	3.151(3)
	MEAN	2.065		O(2)	2.775(3)
			O(7) --	F	2.780(1)
				O(2)	3.015(2)
				MEAN	2.901
Mg(2)	O(1)	2.131(2)	O(7) --	O(1)	2.860(2)
	F	2.013(1)		F	2.609(2)
	O(5)	2.114(2)		O(5)	3.199(1)
	O(6)	2.091(2)		O(6)	3.032(1)
	O(7)	2.075(1)	O(8) --	O(1)	2.807(2)
	O(8)	2.075(2)		F	2.971(1)
	MEAN	2.083		O(5)	2.922(3)
				O(6)	3.132(2)
			O(1) --	F	3.023(2)
				O(5)	2.981(3)
			O(6) --	F	2.863(1)
				O(5)	2.940(2)
				MEAN	2.945

Tetrahedral Sites

S	O(1)	1.481(2)	O(1) --	O(1)	2.412(4)
	O(2)	1.477(2)		O(2)	2.413(2)
	O(3)	1.454(2)		O(3)	2.399(2)
	MEAN	1.476	O(2) --	O(3)	2.397(3)
				MEAN	2.406
B	O(4)	1.441(3)	O(4) --	O(5)	2.407(2)
	O(5)	1.502(4)		O(6)	2.367(2)
	O(6)	1.473(3)		O(8)	2.342(2)
	O(8)	1.467(3)	O(5) --	O(6)	2.429(2)
	MEAN	1.471		O(8)	2.411(3)
			O(6) --	O(8)	2.452(2)
				MEAN	2.401

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[1] To obtain a copy of Table 3, order document AM 82-212 from the Business Office, Mineralogical Society of America, 2000 Florida Avenue N. W., Washington, D. C. 20009. Please remit $1.00 in advance for the microfiche.

Table 5. Distances and angles about the hydrogen atoms and the hydrogen bonding distances and angles.

oxygen	hydrogen	distance	cation-oxygen-hydrogen			angle
O(4)	H(2)	0.78(4)A	B	O(4)	H(2)	111(3)°
O(5)	H(1)	0.74(3)	Mg(1)	O(4)	H(2)	112(3)
O(6)	H(3)	0.70(5)	B	O(5)	H(1)	108(3)
O(7)	H(5)	0.62(4)	Mg(2)	O(5)	H(1)	120(3)
O(8)	H(4)	0.69(4)	B	O(6)	H(3)	113(3)
			Mg(2)	O(6)	H(3)	112(3)
			B	O(8)	H(4)	115(4)
			Mg(2)	O(8)	H(4)	114(4)
			Mg(1)	O(7)	H(5)	105(5)
			Mg(2)	O(7)	H(7)	104(6)

hydrogen bonding

donor	acceptor	distance	donor-H-receptor angle
O(4)	O(5)	2.678A	171(4)°
O(6)	O(2)	3.164	160(4)
O(5)	O(1)	2.837	166(4)

closer apices forming an edge of the sulphate tetrahedron and the separated apices forming part of the boron tetrahedron on either side of the mirror plane.

The Mg-anion as well as the anion–anion distances indicate considerable distortion brought about by the sharing of corners and edges among the octahedra (Table 4). The S–O distances are all very similar as are the edge lengths of the tetrahedron. The B–O distances are more variable as are the edge lengths. Table 6 shows the electrostatic charge balance in the structure with B–O strengths calculated according to Zachariasen (1963).

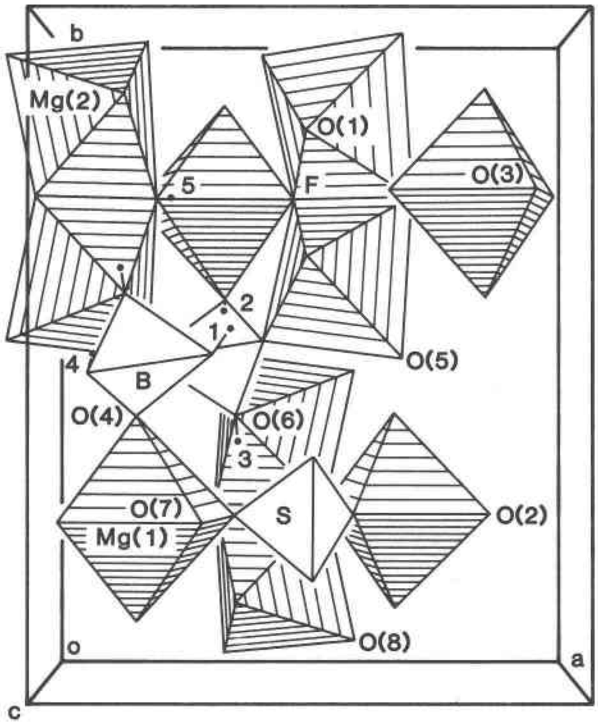

Fig. 1. A perspective view down the *c*-axis of the major units in sulfoborite. Hydrogen atoms are shown as filled circles connected by straight lines to their hydroxyl hydrogens.

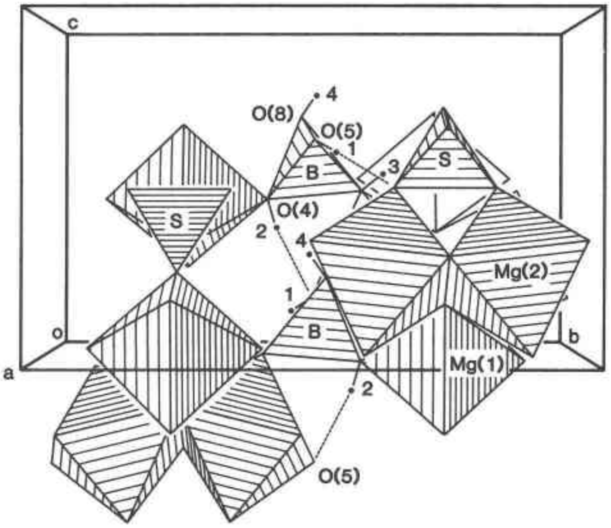

Fig. 2. A perspective view down the *a*-axis showing the hydrogen bonding between O(4)–H(2) and O(5)– and between O(5)–H(1) and O(1). The hydrogen bonds are indicated by dashed lines.

Hydrogen bonding

Since the hydrogen atoms were located during the refinement, the hydrogen bonding scheme can be examined directly. The four hydrogen atoms associated with the boron tetrahedron are shown in Figures 1 and 2 with the dotted lines indicating the hydrogen bonds. For all hydroxyls coordinating boron, as for example in the structure of kernite (Cooper *et al.*, 1973), the B–O–H angle is within a few standard deviations of the tetrahedral angle of 109.47°. This is also true for the Mg–O–H angles in sulfoborite (Table 5). In order for hydrogen bonding

Table 6. Electrostatic charge balance in sulfoborite

	B	S	Mg(1)	Mg(2)	H	H-bond	Sum
O(1)		1.50		0.33			2.01
O(2)		1.50	0.33			0.08	1.91
O(3)		1.50	0.33				1.83
O(4)*	0.84		0.33		0.75		1.92
O(5)*	0.69			0.33	0.82	0.25	2.09
O(6)*	0.74			0.33	0.92		1.99
O(7)*			0.33	0.67	1.00		2.00
O(8)*	0.76			0.33	1.00		1.99
F			0.33	0.67			1.00
						Total	16.84

* hydroxyl

to occur, there must be a receptor atom situated somewhere on or near the surface of a cone of half angle (180–109)/2° whose axis is the vector from the cation to the hydroxyl oxygen. When two cations coordinate one hydroxyl, the geometry is such that the two cones situated about each cation–oxygen vector and having a common apex (the hydroxyl oxygen) must intersect each other and each line of intersection is a possible hydrogen bond direction. For one coordinating cation there is an infinite number of possible bonding directions on the surface of the cone. For two coordinating cations, there will be at most two possible directions, and for three coordinating cations all three cones will intersect (or nearly so) in a single common direction. For three of the five hydroxyls in the structure there is a suitable receptor oxygen and two of these form hydrogen bonds. The third receptor, O(2), is too far away to be considered a hydrogen bond (O(6). . . .O(2) = 3.164Å).

An unusual case is the hydroxyl bond O(7)–H(5). The hydroxyl is coordinated by three magnesium ions as is the fluorine. The electrostatic requirements for the anions are identical and the Mg–anion distances are not significantly different. Why does one site contain hydroxyl and the other fluorine? A close inspection of the cations around O(7) and F shows a distinct difference not in terms of distances but of angles. If one plots the positions of the cations and anion for the hydroxyl and fluorine (Fig. 3), it is immediately apparent that fluorine lies nearly in the plane defined by the three coordinating Mg ions while the hydroxyl oxygen is considerably displaced (0.528Å). This is a direct result of the undulating nature of the chain of octahedra referred to earlier. The hydroxyl occurs where the chain curves outward and the fluorine occupies the inward curving part of the chain.

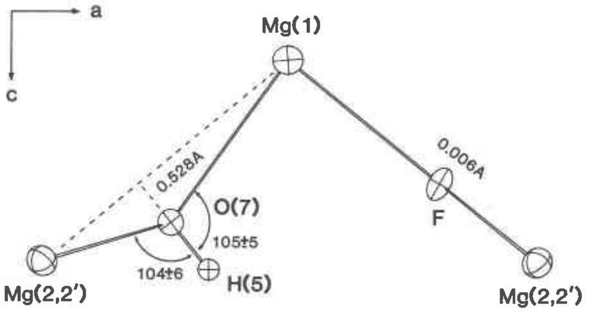

Fig. 3. The environments about F and O(7)–H(5) are shown in a projection down the *b*-axis. All atoms lie in a mirror plane except Mg(2,2′) which are above and below the plane. The distances shown in the figure are the displacements of the F and O(7) from the planes formed by the three Mg atoms. The F is very nearly in this plane while O(7) is considerably displaced. The displacement of O(7) allows Mg–O–H angles which are close to tetrahedral.

The result of this is that in the case of the OH, all Mg–O–H angles are close to tetrahedral: that is, all three cones have intersections which are nearly colinear. There could not possibly be tetrahedral angles in the site occupied by the fluorine since it is coplanar with the three coordinating magnesiums. The inference is that the cation–oxygen–hydrogen angle must be tetrahedral and where this is not possible another anion with charge −1 will preferentially occupy the site. This would explain the ordered arrangement of OH and F in sulfoborite.

The structure as described by Iorysh *et al.* (1976) is in general agreement with our refinement except for small differences in positional parameters due to the less accurate measurement of intensities in their study. This resulted in the identification of fluorine as hydroxyl and the inability to locate hydrogen atoms and thus to identify hydrogen bonding. One might question whether the sulfoborite crystal examined by Iorysh *et al.* and the one used for the present work are chemically different, one having fluorine and the other not. Since neither study included a chemical analysis, this is impossible to answer, but the stereochemical arguments presented in the previous paragraph strongly suggest that fluorine (with perhaps other halogens) is an essential part of the structure. In view of the difficulty in identifying fluorine in an X-ray structure refinement, one wonders if other structures have been reported in the literature in which fluorine has similarly been overlooked and treated as hydroxyl.

Conclusions

Sulfoborite contains octahedrally coordinated magnesium and tetrahedrally coordinated boron and sulfur. All the water is in the form of hydroxyl. Fluorine occupies a single anion site similar in coordination to another site occupied by hydroxyl. The two sites differ in that the hydroxyl is situated such that three M–O–H angles close to the tetrahedral value are possible while the fluorine site cannot accommodate such an arrangement. The sulfoborite formula based on the crystal structure refinement is $Mg_3SO_4(B(OH)_4)_2(OH)F$.

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