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Surinamite, *ca.* $Mg_3Al_4Si_3BeO_{16}$: its crystal structure and relation to sapphirine, *ca.* $Mg_{2.8}Al_{7.2}Si_{1.2}O_{16}$

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Abstract

Surinamite is monoclinic, space group $P2/n$, with $a = 9.916(1)$, $b = 11.384(1)$, $c = 9.631(1)$Å, $\beta = 109.30(1)°$. The asymmetric unit contains *ca.* $Mg_3Al_4Si_3BeO_{16}$ comprised of nine octahedral cations and five tetrahedral cations incorporated in a cubic close-packed array of sixteen independent oxygen atoms. $R = 0.047$ for 2998 independent reflections.

The structure consists of octahedral walls running parallel to x which are connected along y by an open branched chain $^1_\infty[T_5O_{15}]$where one of the tetrahedra, T(1), is principally occupied by Be^{2+}. This tetrahedron is unique in the asymmetric unit in that three of its vertices are shared by other tetrahedra.

Following along [001] in sapphirine and [100] in surinamite, the thicknesses of octahedra and tetrahedra along the [010] direction are:

	sapphirine	surinamite
M	4 · 4 · 3 · 3 ·	3 · 3 · 3 · 2
T	1 · 1 · 2 · 2 ·	1 · 1 · 1 · 2

Introduction

Surinamite is a recent addition to the high-pressure granulite facies minerals, and was described by de Roever *et al.* (1976) from the Bakhuis Mountains, Surinam. The chemical composition, done by electron microprobe, presented a low total for the observed oxides, and they suggested possible presence of $(OH)^-$ groups in the structure. Extreme conditions of formation and close chemical and physical similarity to sapphirine were other reasons suggested for its rarity. But low oxide totals persisted in reports on new finds, Woodford and Wilson (1976) offering 97.05% oxide sum for an Australian occurrence. Recently, de Roever *et al.* (1981) resolved the problem. They failed to synthesize the phase in the system Mg–Fe–Al–Si–O–H but detected the presence of Be (4–5 wt.% BeO) by ARL ion microprobe analysis and atomic absorption spectrophotometric analysis on material from the type locality. Finally, they synthesized the phase in the system Mg–Fe–Al–Be–Si–O–H at 20 kbar and 800°C, and proposed the formula $(Mg,Fe)_3(Al,Fe)_4[BeSi_3O_{16}]$ which is confirmed in the present study. Since Grew (1981) independently reached the same conclusion, these findings then cast doubt on the crystal-chemical study by Moore (1976). Our present study appears to resolve these conflicts.

In addition, several crystallographic problems elicited our interest. Merlino (1973, 1980) demonstrated the appearance of order–disorder structures for sapphirines (which are structurally allied to surinamite). Merlino discussed order–disorder in terms of the fundamental study by Dornberger-Schiff (1956) on such structures. Since Moore (1976) merely proposed a structure for surinamite, order–disorder remained a possibility and when single crystals became available, a three-dimensional structure refinement appeared desirable.

Experimental

Several grains of Christmas Point, Antarctica surinamite were kindly submitted to us by Edward S. Grew of UCLA. The chemistry and paragenesis of these grains were described by Grew (1981) in sample No. 2292C. Earlier, Moore (1976) derived cell contents and cell parameters from a tiny (40 μm) grain from the type locality in high-grade metamorphic rocks from the Bakhuis Mountains, western Surinam (De Roever *et al.*, 1976). To compare it with sapphirine, Moore earlier suggested $M_{60}T_{40}O_{160}$ for surinamite, where M = octahedrally coordinated and T = tetrahedrally coordinated cations by oxygen anions. With essential beryllium, our structure study leads to $M_{60}T_{50}O_{160}$ for the same oxygen stoichiometry as above. Our cell contents are $M_{24}T_{20}O_{64}$ for surinamite. Scaling by a factor of 2.5, it is clear that the absence of one tetrahedral occupancy (equipoint rank number 4 for a general position) leads to exactly Moore's (1976) proposed stoichiometry. Clearly, the culprit was earlier absence of the light element beryllium!

Actually, there is another flaw in Moore's (1976) study: the proposed structure cell is wrong. Due to the extremely small size of the type crystal, the Weissenberg photographs had to be exposed for four days each, and weak systematic superstructure reflections were not discernible due to the backscatter. The present and the earlier

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data are as follows:

	Surinamite This Study	Surinamite Old	Surinamite New	Sapphirine Old	Sapphirine New
a(Å)	9.916(1)	9.64	9.90	11.266	9.929
b(Å)	11.384(1)	11.36	11.36	14.401	14.401
c(Å)	9.631(1)	4.95	9.64	9.929	9.783
β(deg.)	109.30(1)	109.0	109.0	125.46	110.28
Space group	$P2/n$	$P2_1/a$	---	$P2_1/a$	$P2_1/n$
Transform	--	[2×001/010/$\bar{1}$00]		[001/0$\bar{1}$0/101]	
Reference	--	Moore (1976)	---	Moore (1969)	--

The refined single crystal unit cell data used in this study were obtained by several low, intermediate and high angle reflections on the Picker FACS-1 automated diffractometer, also used for the intensity data collection.

A single grain from Christmas Point, Enderby Land, Antarctica was used throughout this study. It measured 0.3 mm ||[100] × 0.04 mm ||[010] × 0.06 mm ||[001]. Reflection of the type (*hkl*) and (*hk̄l*) were collected up to $\sin\theta/\lambda = 0.70$. The crystal was not quite regular in shape; the intensity distribution of equivalent reflections and relatively low linear atomic absorption coefficient, $\mu = 1.12$ cm^{-1} for MoK_α radiation, led us to conclude that absorption correction was unnecessary. Over 4500 reflections were collected on a Picker diffractometer, graphite monochromatized MoK_α radiation of 50 kV and 20 mA, scan rate 2° min^{-1}. Reference reflections were monitored throughout to assess machine stability. Measured intensities were then corrected for Lorentz and polarization factors, and averaged to yield 2998 independent reflections.

The structure was solved in stages by Patterson synthesis and successive Fourier syntheses, with knowledge of the sapphirine structure (Moore, 1969). Scattering curves for Be^{2+}, Mg^{2+}, Fe^{2+}, Al^{3+}, Si^{4+} and O^{1-} were obtained from *International Tables* (1974) and anomalous dispersion correction for all heavier metals from Cromer and Liberman (1970). Final refinement converged to $R = 0.047$ for all 2998 independent reflections and 0.029 for 2093 reflections above 3σ of background error where

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

Refinement minimized $w(F_o - F_c)^2$. Refined variables included the scale factor, isotropic secondary extinction ($2.2(1) \times 10^{-7}$), atomic coordinate parameters (77 parameters), varied site occupancy parameters (8 parameters) and anisotropic thermal vibration parameters (170 parameters), giving a total of 257 varied parameters, or an independent data to variable parameter ratio of 11.9:1. The final atomic coordinate parameters for surinamite are given in Table 1. Table 2 outlines some chemical analyses of surinamite and beryllium-bearing sapphirine reported in Grew's study on material from Enderby Land, and some calculations from the structure refinement and hypothetical end-member formulae. Table 3 presents the anisotropic thermal vibration parameters and Table 4 the observed and calcualted structure factors.[1] Table 5 attempts to demonstrate that the proposed anion packing of Moore (1976) is essentially confirmed. The bond distance and angle calculations are given in Table 6.

The model proposed by Moore (1976) for the idealized fractional anion coordinates of surinamite is basically correct but it is not immediately obvious. In that paper, it was considered imprudent to propose cation positions but it was stated that the octahedral cations are distributed at levels $z = 0$, 1/4, 1/2 and 3/4 (orientation of this study). As mentioned earlier, the small grain from the type locality yielded a paucity of data. Our present study requires first, a cell transformation from old to new, [001]/[010]/[$\bar{1}$00], to bring Moore (1976) in conformity with the present results. It was also noted that the strongest reflection for $h \neq 2n$ is ($\bar{3}$03) with $|F_o| = 96.5$. The strongest reflection of the entire data set is (404) with $|F_o| = 440.3$, and its intensity differs by a factor of *twenty* from $h \neq 2n$ reflections. Since $P2/n$ is neither a sub- nor supergroup of $P2_1/c$, proof that the proposed model agrees with the present included a list of all equivalences in $P2/n$ for O(1)–O(16) of this study, and a list of all equivalences in $P2_1/c$ for O(1)–O(8) in Moore (1976). These were found to match a subset of the $P2/n$ tabulation. The remaining 32 positions were related by (x − 1/2), (y), (z) of the tabulations of entries and were a consequence of doubling the transformed *a* axis of the former study. This observation is summarized in Table 5.

Discussion of the structure

The crystal structure of surinamite is represented as a polyhedral diagram of the actual structure projected down c^* in Figure 1, and as an idealization in Figure 2. They have been drawn so that direct comparison with Figures 1 and 3 in Moore (1969) are possible.

Both surinamite and sapphirine have in common a structural principle based on cubic close-packing of the oxide anions. Selecting sapphirine's cell in Moore (1969) and surinamite's cell in this study, the former has cubic close-packed layers stacked parallel to {100} and the latter has such layers stacked parallel to {001}. Four layers comprise the cell repeats in these directions. The two structure types can be compared more specifically.

	sapphirine		surinamite	
	a sinβ	9.18 Å	c sinβ	9.09 Å
	layer repeat	2.30 Å	layer repeat	2.27 Å
	V/O^{2-}	16.40 Å^3	V/O^{2-}	16.03 Å^3
Formula (16 O^{2-})	$Mg_{2.8}Al_{7.2}Si_{1.2}O_{16}$		$Mg_3Al_4Si_3BeO_{16}$	
Formula (Z = 2)	$M_{14}(M_2)O_4[T_{12}O_{36}]$		$M_{11}(M)O_2[T_{10}O_{30}]$	
M:T	1.33		1.20	

[1] To obtain a copy of Table 4, order Document AM-83-227 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 1. Surinamite: atomic coordinate parameters†

Atom	Occupancy	Equipoint	x	y	z
M(1)	0.589(3) Mg^{2+} + 0.411 Fe^{2+}	4	0.47718(6)	0.65733(5)	0.25876(7)
M(2)	0.853(3) Al^{3+} + 0.147 Fe^{2+}	4	0.50124(7)	0.37756(6)	0.26827(8)
M(3)	0.946(3) Al^{3+} + 0.054 Fe^{2+}	4	0.50226(8)	0.11446(6)	0.25443(8)
M(4)	1.000 Al^{3+}	2	0.25000	0.25314(11)	0.25000
M(5)	0.957(4) Mg^{2+} + 0.043 Fe^{2+}	2	0.25000	0.96665(10)	0.25000
M(6)	1.000 Al^{3+}	2	0.75000	0.51164(10)	0.25000
M(7)	0.799(4) Mg^{2+} + 0.201 Fe^{2+}	2	0.75000	0.25546(9)	0.25000
M(8)	0.950(4) Mg^{2+} + 0.050 Fe^{2+}	2	0.75000	0.97460(10)	0.25000
M(9)	1.000 Al^{3+}	2	0.00000	0.50000	0.50000
T(1)	0.945(4) Be^{2+} + 0.055 Si^{4+}	4	0.32307(30)	0.75235(24)	0.45592(31)
T(2)	1.000 Si^{4+}	4	0.07671(8)	0.88380(7)	0.44821(8)
T(3)	1.000 Si^{4+}	4	0.30678(8)	0.50165(7)	0.43709(8)
T(4)	1.000 Si^{4+}	4	0.56917(8)	0.88011(7)	0.44754(8)
T(5)	0.941(3) Al^{3+} + 0.059□	4	0.82994(8)	0.74462(7)	0.45244(9)
O(1)		4	0.11631(18)	0.99878(17)	0.37095(19)
O(2)		4	0.61382(18)	0.99424(17)	0.37191(19)
O(3)		4	0.87706(19)	0.11366(16)	0.37042(20)
O(4)		4	0.37628(19)	0.11562(16)	0.37104(20)
O(5)		4	0.90335(19)	0.86355(16)	0.38761(20)
O(6)		4	0.39954(19)	0.85556(16)	0.38810(20)
O(7)		4	0.61041(19)	0.24671(16)	0.36210(20)
O(8)		4	0.64425(19)	0.76573(16)	0.39752(20)
O(9)		4	0.10811(19)	0.25065(17)	0.35473(20)
O(10)		4	0.14913(19)	0.76935(16)	0.40286(20)
O(11)		4	0.35898(19)	0.62573(16)	0.39176(21)
O(12)		4	0.37027(19)	0.39285(16)	0.36854(21)
O(13)		4	0.88120(19)	0.61981(16)	0.37314(20)
O(14)		4	0.88412(19)	0.40015(15)	0.35382(21)
O(15)		4	0.63209(18)	0.50572(18)	0.37948(20)
O(16)		4	0.12767(18)	0.49848(18)	0.38191(19)

†Estimated standard errors refer to the last digit.

It is seen that surinamite is a little more efficiently packed than sapphirine, as expected for a mineral which has a higher proportion of tetrahedral population, more Si^{4+} and the presence of Be^{2+}. The general formulae based on two "molecules" in the cell express the octahedral (M) and tetrahedral (T) populations. The octahedral populations which occur between the octahedral walls (which run parallel to [001] in sapphirine and [100] in surinamite) share all basal edges with the walls above and below. In surinamite, this corresponds to M(9) which is fixed at an

Table 2. Surinamite and beryllian sapphirine: chemical analyses and interpretation

	1	2	3	4	5
BeO	[3.5]	4.72	4.27	2.2-2.5	3.71
MgO	16.5	22.82	14.11	15.45-15.48	17.95
MnO	0.2	---	---	0.01-0.03	---
FeO	13.0	---	9.76	9.9-10.1	---
Al_2O_3	33.8	38.46	38.89	50.7-51.1	60.51
SiO_2	31.1	34.00	32.97	19.2-20.3	17.83
H_2O	0.66 ± 0.2	---	---	---	---
Total	99.0	100.00	100.00		100.00

[1]Average of two Christmas Point analyses in Grew (1981). According to the author, BeO content was assumed in the deficiency reported in earlier electron microprobe analysis. See Grew for this and water determination. Included are 0.03 TiO_2, 0.01 Cr_2O_3, 0.06 ZnO, 0.09 CaO, 0.01 Na_2O and 0.02 K_2O. A portion of this sample resides in the Smithsonian Institution, USNM 147434.

[2]For hypothetical $Mg_3Al_4Si_3BeO_{16}$.

[3]Calculated from cell contents in Table 1.

[4]Grew (1981) for Zircon Point sapphirine. Also 0.01 TiO_2, 0.02 Cr_2O_3, 0.10 ZnO, 0.05-0.15 CaO, 0.03-0.04 K_2O.

[5]For hypothetical $Mg_3Al_8Si_2BeO_{20}$.

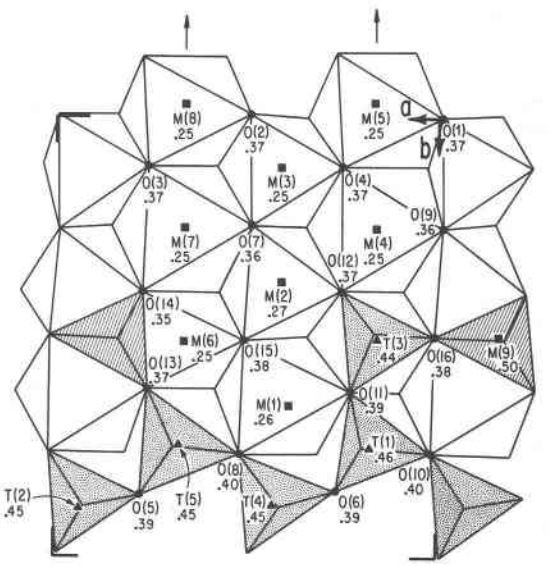

Fig. 1. Polyhedral diagram of the surinamite structure down z^* between $0 < z < 1/2$. Octahedra in the walls are unshaded and the tetrahedra are stippled. The M(9) octahedron between the walls resides above the ruled region. Compare with Fig. 1 in Moore (1969).

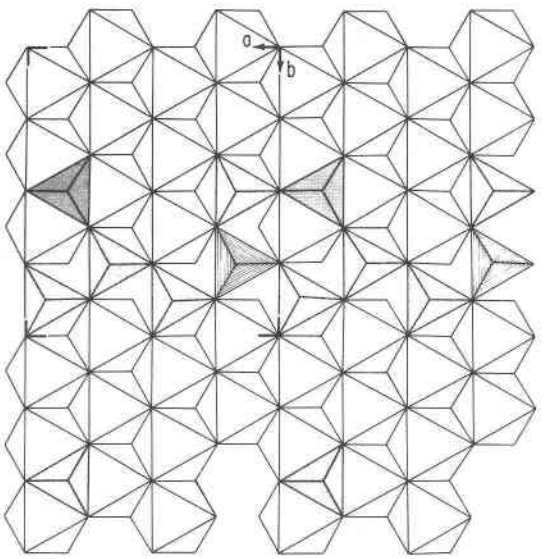

Fig. 2. Idealized polyhedral diagram of the surinamite crystal structure down z^*. The octahedral walls are unshaded, the (Si,Al)–O tetrahedra are stippled and the Be (= T(1))–O tetrahedra are ruled. The M(9) octahedra between the walls reside above the shaded regions. Tetrahedra below the walls are not shown. The surinamite cell is outlined.

inversion center. Both structures are based on T_nO_{3n} tetrahedral chains which are pyroxene-like chains with "wings". In fact, according to the branched anion classification of silicates by Liebau (1978), both sapphirine and surinamite have *open branched vierer single chains*. Later, distinction will be made between sapphirine and surinamite on the basis of the branches.

A convenient description for both structures is to match the relative thicknesses of octahedral walls and tetrahedral "wings" or branches. This can be achieved by following along [001] and [100] in sapphirine and surinamite respectively and counting the number of octahedra and tetrahedra along the [010] direction. We see that the octahedral wall in sapphirine has four edge-sharing octahedra successively followed by four, three, and three similar ones. The corresponding tetrahedral portion is one, one, two, two. Stated briefly:

	sapphirine	surinamite
M	4 · 4 · 3 · 3 ·	3 · 3 · 3 · 2
T	1 · 1 · 2 · 2 ·	1 · 1 · 1 · 2

In effect the extent of lateral branching is being compared between two structures based on oxide cubic close packing. Note that the octahedral walls and the tetrahedral branches are wider in sapphirine than in surinamite. But beyond this, there does not appear to be any simple way to predict other articulations of branches and walls which may exist as stable phases. But the structural relations between sapphirine and surinamite do emphasize the caution that would be required to distinguish natural and synthetic phases which resemble sapphirine and surinamite.

Table 3. Surinamite: anisotropic thermal vibration parameters†

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}	B_{eq}
M(1)	72(3)	93(3)	72(3)	-11(2)	35(2)	2(2)	0.60
M(2)	60(3)	66(3)	75(4)	- 3(3)	35(3)	- 3(3)	0.51
M(3)	54(4)	55(4)	59(4)	- 1(3)	27(3)	4(3)	0.43
M(4)	85(6)	108(6)	108(6)	0	50(5)	0	0.75
M(5)	37(6)	63(6)	65(6)	0	27(5)	0	0.41
M(6)	64(5)	87(6)	71(5)	0	20(4)	0	0.59
M(7)	46(5)	55(5)	96(6)	0	45(4)	0	0.47
M(8)	38(6)	58(6)	63(6)	0	27(5)	0	0.40
M(9)	48(5)	78(5)	59(5)	- 2(4)	17(4)	1(4)	0.49
T(1)	62(14)	63(14)	62(15)	- 5(10)	22(11)	4(11)	0.49
T(2)	73(3)	84(4)	71(4)	- 0(3)	32(3)	1(3)	0.58
T(3)	74(3)	96(3)	70(3)	- 2(3)	29(3)	2(3)	0.62
T(4)	74(3)	78(4)	66(4)	3(3)	29(3)	- 1(3)	0.56
T(5)	51(4)	47(4)	43(4)	3(3)	22(3)	- 3(3)	0.36
O(1)	72(9)	88(9)	88(9)	- 1(7)	38(7)	7(8)	0.63
O(2)	79(9)	87(9)	89(9)	5(7)	37(7)	10(8)	0.65
O(3)	73(9)	92(9)	75(10)	- 2(7)	32(7)	3(7)	0.62
O(4)	73(9)	87(9)	74(10)	- 2(7)	26(7)	3(7)	0.61
O(5)	70(9)	86(9)	85(10)	- 3(7)	23(7)	12(7)	0.64
O(6)	71(9)	108(10)	76(10)	-11(7)	22(7)	14(7)	0.68
O(7)	73(9)	100(10)	83(9)	- 7(7)	35(7)	14(8)	0.66
O(8)	80(9)	88(10)	105(10)	2(7)	37(8)	-8(7)	0.71
O(9)	72(9)	110(10)	71(9)	- 1(7)	25(7)	0(7)	0.66
O(10)	87(9)	95(10)	101(10)	2(7)	41(8)	-15(7)	0.72
O(11)	91(9)	104(9)	94(10)	-10(7)	35(7)	5(8)	0.75
O(12)	84(9)	129(10)	79(10)	- 1(7)	17(8)	- 8(8)	0.79
O(13)	72(9)	96(9)	75(10)	0(7)	26(7)	- 1(8)	0.64
O(14)	77(9)	98(9)	71(9)	- 8(7)	29(7)	- 4(7)	0.64
O(15)	85(9)	109(10)	96(9)	11(8)	37(7)	- 5(8)	0.75
O(16)	90(9)	111(10)	91(9)	- 4(8)	36(7)	- 4(8)	0.73

†Coefficients in the expression $\exp-[U_{11}h^2 + U_{22}k^2 + U_{33}\ell^2 + 2U_{12}hk + 2U_{13}h\ell + 2U_{23}k\ell]$. The equivalent isotropic thermal parameter, B_{eq}, is also listed. Estimated standard errors refer to the last digit except for those coefficients related by symmetry. The coefficients are $\times 10^4$.

Is it possible to interpret the chemical composition of surinamite on the basis of the refined crystal structure? The equivalent isotropic thermal parameters in Table 3 suggest a structure which is not only based on dense-packed oxide anions but also has a minimum of stacking disorder and domain structure. With $B_{eq} = 0.36\text{Å}^2$ for T(5) representing the lowest value in Table 3, we hold 0.059□ for T(5) in Table 1 with some doubt. This small

Table 5. Surinamite: comparison of earlier proposed anion coordinates with present study†

	n/8	Entries				Moore (1976)			
Atom	x y z	x y z	$\bar{x}\ \bar{y}\ \bar{z}$	½-x y ½-z	½+x $\bar{y}$ ½+z	Atom	x	y	z
O(1)	1 0 3	O(2)*	O(2)*	O(1)	O(1)	O(1)	3	0	1
O(2)	5 0 3	O(3)	O(3)	O(1)*	O(1)*	O(2)	3	2	1
O(3)	7 1 3	O(7)	O(7)	O(4)*	O(4)*	O(3)	3	4	1
O(4)	3 1 3	O(3)*	O(3)*	O(5)	O(5)	O(4)	3	6	1
O(5)	7 7 3	O(6)	O(6)	O(6)*	O(6)*	O(5)	1	1	1
O(6)	3 7 3	O(8)	O(8)	O(8)	O(8)	O(6)	1	3	1
O(7)	5 2 3	O(4)	O(4)	O(9)*	O(9)*	O(7)	1	5	1
O(8)	5 6 3	O(2)	O(2)	O(10)*	O(10)*	O(8)	1	7	1
O(9)	1 2 3	O(7)*	O(7)*	O(2)	O(2)	$P2_1/c$ setting:			
O(10)	1 6 3	O(8)*	O(8)*	O(4)	O(4)	x y z	$\bar{x}$	½+y	½-z
O(11)	3 5 3	O(13)*	O(13)*	O(7)	O(7)	$\bar{x}\ \bar{y}\ \bar{z}$	x	½-y	½+z
O(12)	3 3 3	O(14)*	O(14)*	O(6)	O(6)				
O(13)	7 5 3	O(5)	O(5)	O(11)*	O(11)*				
O(14)	7 3 3	O(12)*	O(12)*	O(12)*	O(12)*				
O(15)	5 4 3	O(1)	O(1)	O(16)*	O(16)*				
O(16)	1 4 3	O(15)*	O(15)*	O(3)	O(3)				

†The atom labels are those in this study. The n refers to the nearest integer for coordinates in Table 1 referred to fractional coordinates. The entries are those proposed atom positions for O^{2-} in Moore (1976), but with $P2_1/c$, a = 2 × 4.95, b = 11.36, c = 9.64 Å. The starred labels refer to atom labels in this study related by (x-½), (y), (z).

Table 6. Surinamite: bond distances and angles†

M(1)			M(2)			M(3)		
M(1)-O(11)	2.034(2) Å		M(2)-O(12)	1.865(2)		M(3)-O(2)	1.884(2)	
-O(10)$^{(2)}$	2.081(2)		-O(7)	1.887(2)		-O(1)$^{(2)}$	1.907(2)	
-O(8)	2.142(2)		-O(14)$^{(2)}$	1.904(2)		-O(4)	1.936(2)	
-O(13)$^{(2)}$	2.224(2)		-O(9)$^{(2)}$	1.954(2)		-O(7)	1.938(2)	
-O(16)$^{(2)}$	2.292(2)		-O(15)	2.010(2)		-O(3)$^{(2)}$	1.957(2)	
-O(15)	2.347(2)		-O(16)$^{(2)}$	2.097(2)		-O(9)$^{(2)}$	1.986(2)	
Average	2.187 Å		Average	1.953		Average	1.935	
*O(13)$^{(2)}$-O(15)	2.722(3)	73.04(7)°	*O(7)-O(9)$^{(2)}$	2.463(3)	79.76(9)	*O(7)-O(9)$^{(2)}$	2.463(3)	77.73(9)
*O(13)$^{(2)}$-O(16)$^{(2)}$	2.784(3)	76.09(7)	*O(14)$^{(2)}$-O(15)	2.506(3)	79.57(8)	O(1)$^{(2)}$-O(2)	2.674(3)	89.74(10)
*O(15)-O(16)$^{(2)}$	2.948(3)	78.89(8)	*O(14)$^{(2)}$-O(16)$^{(2)}$	2.594(3)	80.66(9)	*O(1)$^{(2)}$-O(4)	2.705(3)	89.48(9)
O(8)-O(15)	2.965(3)	82.53(8)	O(12)-O(16)$^{(2)}$	2.701(3)	85.75(9)	O(1)$^{(2)}$-O(3)$^{(2)}$	2.708(3)	88.97(9)
O(8)-O(13)$^{(2)}$	3.030(3)	87.87(8)	*O(7)-O(14)$^{(2)}$	2.730(3)	92.14(9)	*O(4)-O(9)$^{(2)}$	2.709(3)	87.33(8)
O(11)-O(16)$^{(2)}$	3.048(3)	89.39(8)	*O(9)$^{(2)}$-O(12)	2.756(3)	92.35(9)	O(2)-O(4)	2.728(3)	91.14(9)
O(11)-O(15)	3.086(3)	88.68(8)	O(9)$^{(2)}$-O(14)$^{(2)}$	2.796(3)	92.89(9)	*O(2)-O(3)$^{(2)}$	2.728(3)	90.50(9)
O(10)$^{(2)}$-O(13)$^{(2)}$	3.088(3)	91.61(8)	O(9)$^{(2)}$-O(16)$^{(2)}$	2.834(3)	88.72(9)	*O(3)$^{(2)}$-O(7)	2.740(3)	89.41(8)
O(10)$^{(2)}$-O(16)$^{(2)}$	3.093(3)	89.89(8)	O(12)-O(15)	2.867(3)	95.38(9)	O(4)-O(7)	2.785(3)	91.91(9)
O(8)-O(11)	3.235(3)	101.35(9)	O(7)-O(12)	2.922(3)	102.31(9)	O(3)$^{(2)}$-O(9)$^{(2)}$	2.817(3)	91.16(9)
O(10)$^{(2)}$-O(11)	3.253(3)	104.46(9)	*O(15)-O(16)$^{(2)}$	2.948(3)	91.72(9)	O(1)$^{(2)}$-O(9)$^{(2)}$	2.871(3)	95.01(10)
O(8)-O(10)$^{(2)}$	3.357(3)	105.30(8)	O(7)-O(15)	2.957(3)	98.67(10)	O(2)-O(7)	2.875(3)	97.57(10)
Average	3.051	89.09	Average	2.756	89.99	Average	2.734	90.00
	T(1)			T(2)			T(3)	
T(1)-O(10)	1.640(3)		T(2)-O(10)	1.616(2)		T(3)-O(11)	1.613(2)	
-O(6)	1.646(3)		-O(1)	1.617(2)		-O(12)	1.625(2)	
-O(11)	1.653(3)		-O(5)	1.639(2)		-O(15)$^{(1)}$	1.669(2)	
-O(7)$^{(1)}$	1.656(3)		-O(3)$^{(1)}$	1.653(2)		-O(16)	1.678(2)	
Average	1.649		Average	1.631		Average	1.646	
O(6)-O(11)	2.649(3)	106.9(2)	O(5)-O(10)	2.622(3)	107.3(1)	O(11)-O(15)$^{(1)}$	2.640(3)	107.1(1)
O(10)-O(11)	2.676(3)	108.7(2)	O(3)$^{(1)}$-O(5)	2.624(3)	105.7(1)	O(11)-O(12)	2.666(3)	110.8(1)
O(7)$^{(1)}$-O(10)	2.697(3)	109.8(2)	O(1)-O(10)	2.637(3)	109.3(1)	O(11)-O(16)	2.688(3)	109.5(1)
O(6)-O(7)$^{(1)}$	2.704(3)	109.9(2)	O(3)$^{(1)}$-O(10)	2.643(3)	107.9(1)	O(12)-O(15)$^{(1)}$	2.694(3)	109.7(1)
O(7)$^{(1)}$-O(11)	2.710(3)	110.0(2)	O(1)-O(5)	2.661(3)	109.6(1)	O(15)$^{(1)}$-O(16)	2.709(3)	108.1(1)
O(6)-O(10)	2.717(3)	111.5(2)	O(1)-O(3)$^{(1)}$	2.782(3)	116.6(1)	O(12)-O(16)	2.730(3)	111.5(1)
Average	2.692	109.5	Average	2.662	109.4	Average	2.688	109.5

†Estimated standard errors in parentheses refer to the last digit. The equivalent positions (referred to Table 1) are designated as superscripts and are (1) = -x, -y, -z; (2) = ½-x, y, ½-z; (3) ½+x, -y, ½+z.

*Shared octahedral edges.

proposed vacancy may indeed not exist, in which case all sites would be fully occupied in the structure. Initially, it was hoped to derive approximate site populations through ionic radii of Mg^{2+}, Al^{3+} and Si^{4+} as was done for sapphirine by Moore (1969). Unfortunately, surinamite contains substantial Fe^{2+} and Be^{2+} as well (Table 2). Therefore, mixed scattering curves were used involving $(Mg_x^{2+}Fe_{1-x}^{2+})$ and $(Al_y^{3+}Fe_{1-y}^{2+})$. For T(1), the mixed curve $(Be_z^{2+}Si_{1-z}^{4+})$ was used. Since the scattering factor difference between these pairs is substantial, refinement converged without difficulty. The problem remained with combinations like $(Mg_x^{2+}Al_{1-x}^{3+})$ and $(Al_y^{3+}Si_{1-y}^{4+})$ where such refinement based on X-ray data is not possible. With at least five oxide components present, it was considered inadvisable to proceed any further. Thus, the calculated chemical analysis from refined cell contents (column 3 in Table 2) is only approximate. MgO and FeO, for example, are low while Al_2O_3 is high. This doubtless arises from Mg^{2+} and Fe^{2+} (possibly Fe^{3+}) substitution for Al^{3+} at M(4), since the mean M(4)–O = 2.06Å distance suggests substantial, if not predominant Mg^{2+}, at this site.

Be^{2+} appears to be nearly completely located in T(1). This tetrahedral site is unique in that three of its corners are shared with other tetrahedra, while the others share at most two corners with other tetrahedra. Indeed, the electrostatic balances in Table 7 for the four T(1) oxygens—O(6), O(7), O(10), O(11)—show that all these oxygens are undersaturated with respect to cations and their charges. Again, this table requires caution since the (Mg,Al) substitutions were not considered.

This suggests an interpretation of the Zircon Point sapphirine by Grew (1981), reproduced in column 4, Table 2. This sapphirine contains between 2.2 and 2.5% BeO. Does sapphirine have a similar region in its structure which corresponds to the T(1) site in surinamite? Of the six nonequivalent T sites in sapphirine, T(2) and T(3) are each 3-connected with other tetrahedra. Of these two, only T(2) possesses all four oxygens which are oversaturated and T(2)–O = 1.66Å also represents the smallest average of all six tetrahedra. From this, it is tempting to write $^{[6]}M_8{}^{[4]}(BeT_5)O_{20}$ where Be^{2+} substitutes at T(2). From Moore (1969), a possible composition could be as

Table 6. (continued)

	M(4)			M(5)			M(6)	
2 M(4)-O(9)	1.984(2)		2 M(5)-O(6)	2.065(2)		2 M(6)-O(14)	1.871(2)	
2 -O(12)	2.087(2)		2 -O(1)	2.066(2)		2 -O(13)	1.896(2)	
2 -O(14)	2.101(2)		2 -O(4)	2.199(2)		2 -O(15)	1.972(2)	
Average	2.057		Average	2.110		Average	1.913	
1 O(12)-O(12)$^{(2)}$	2.702(4)	80.70(12)	*2 O(1)-O(4)$^{(2)}$	2.705(3)	78.66(8)	*2 O(14)-O(15)$^{(2)}$	2.506(3)	81.34(9)
*2 O(4)-O(9)$^{(2)}$	2.709(3)	83.03(8)	*1 O(4)-O(4)$^{(2)}$	2.801(4)	79.11(11)	*2 O(13)-O(14)	2.508(3)	83.50(9)
*2 O(9)-O(12)$^{(2)}$	2.756(3)	85.18(8)	2 O(1)-O(4)	2.900(3)	85.62(8)	*2 O(13)-O(15)$^{(2)}$	2.722(3)	89.43(9)
*1 O(4)-O(4)$^{(2)}$	2.801(4)	83.64(12)	2 O(1)-O(6)$^{(2)}$	2.941(3)	90.78(8)	*1 O(14)-O(14)$^{(2)}$	2.749(4)	94.56(13)
2 O(9)-O(12)	3.028(3)	96.08(9)	2 O(4)-O(6)	2.970(3)	88.22(8)	2 O(13)-O(15)	2.809(3)	93.12(9)
2 O(4)-O(9)	3.030(3)	95.74(8)	2 O(1)-O(6)	3.204(3)	101.73(8)	2 O(14)-O(15)	2.856(3)	95.98(9)
2 O(4)-O(12)	3.156(4)	97.84(8)	1 O(6)-O(6)$^{(2)}$	3.264(3)	104.46(12)	1 O(13)-O(13)$^{(2)}$	2.884(4)	99.00(13)
Average	2.905		Average	2.959	89.47	Average	2.703	90.03
	M(7)			M(8)			M(9)	
2 M(7)-O(7)	2.100(2)		2 M(8)-O(2)	2.074(2)		2 M(9)-O(14)	1.877(2)	
2 -O(3)	2.138(2)		2 -O(5)	2.082(2)		2 -O(13)	1.947(2)	
2 -O(14)	2.145(2)		2 -O(3)	2.115(2)		2 -O(16)	1.962(2)	
Average	2.128		Average	2.090		Average	1.929	
*2 O(7)-O(14)$^{(2)}$	2.730(3)	81.85(8)	*2 O(2)-O(3)$^{(2)}$	2.728(3)	81.28(8)	*2 O(13)-O(14)	2.508(3)	81.96(9
*2 O(3)-O(7)$^{(2)}$	2.740(3)	82.39(8)	*1 O(3)-O(3)$^{(2)}$	2.805(4)	83.07(11)	*2 O(14)-O(16)	2.594(3)	84.97(9)
*1 O(14)-O(14)$^{(2)}$	2.749(4)	79.69(11)	2 O(3)-O(5)	2.859(3)	85.88(8)	2 O(13)-O(16)$^{(1)}$	2.743(3)	89.14(8)
*1 O(3)-O(3)$^{(2)}$	2.805(4)	81.96(11)	2 O(2)-O(5)$^{(2)}$	2.865(3)	87.17(8)	*2 O(13)-O(16)	2.784(3)	90.86(8)
2 O(7)-O(14)	3.251(4)	102.57(8)	2 O(2)-O(3)	2.947(3)	89.44(8)	2 O(14)-O(16)$^{(1)}$	2.832(3)	95.03(9)
2 O(3)-O(14)	3.267(4)	99.41(8)	2 O(2)-O(5)	3.192(4)	100.39(8)	2 O(13)$^{(1)}$-O(14)	2.887(3)	98.04(9)
2 O(3)-O(7)	3.272(4)	93.32(8)	1 O(5)-O(5)$^{(2)}$	3.308(4)	105.23(12)	Average	2.725	90.00
Average	3.006	90.06	Average	2.941	89.72			
	T(4)			T(5)				
T(4)-O(6)	1.612(2)		T(5)-O(5)	1.747(2)				
-O(2)	1.621(2)		-O(9)$^{(1)}$	1.753(2)				
-O(8)	1.649(2)		-O(8)	1.756(2)				
-O(4)$^{(1)}$	1.650(2)		-O(13)	1.766(2)				
Average	1.633		Average	1.756				
O(6)-O(8)	2.607(3)	106.2(1)	O(5)-O(13)	2.783(3)	104.8(1)			
O(2)-O(8)	2.621(3)	106.6(1)	O(8)-O(9)$^{(1)}$	2.808(3)	106.3(1)			
O(4)$^{(1)}$-O(6)	2.650(3)	108.6(1)	O(5)-O(8)	2.831(3)	107.8(1)			
O(4)$^{(1)}$-O(8)	2.671(3)	108.1(1)	O(5)-O(9)$^{(1)}$	2.837(3)	108.3(1)			
O(2)-O(6)	2.693(3)	112.8(1)	O(8)-O(13)	2.950(3)	113.8(1)			
O(2)-O(4)$^{(1)}$	2.746(3)	114.2(1)	O(9)$^{(1)}$-O(13)	2.978(3)	115.6(1)			
Average	2.665	109.4	Average	2.865	109.4			

column 5, Table 2. This composition is not far from the analysis of Grew (1981) in column 4, Table 2. We have secured some beryllian sapphirine grains from Professor Grew, in hopes of exploring this problem through structure refinement.

Liebau (1978) has presented a classification scheme for the silicates which spans a wide variety of structural information. In this classification, he distinguishes between solid solution of Si^{4+} with some other tetrahedrally coordinated cation, from ordered tetrahedral sites occupied by cations other than Si^{4+}, such as tetrahedral Fe^{3+}, Zn^{2+}, Be^{2+} and Li^{1+}. For surinamite, if Be^{2+} is included in the tetrahedral anionic group, then it would be $^{0B}{}^{1}_{\infty}[T_4BeO_{15}]$ where T implies (Si,Al) solid solution. It would be an open branched *vierer* single chain. Excluding the Be^{2+} cation, surinamite would be a mixed anion silicate, with TO_4 and T_3O_{10} oligosilicate units. This would relate it to kilchoanite and ardennite. Sapphirine is likewise based on an open branched *vierer* single chain, and for this reason we prefer to include Be^{2+} in the description of the tetrahedral anionic architecture.

The interatomic distances and angles in Table 6 reveal the cubic close-packed nature of the anion frame and the tendency for shared polyhedral edges to be foreshortened. In cubic close-packing, tetrahedra cannot share edges with octahedra unless these polyhedra actually share faces. Accordingly, no tetrahedra share edges in the structure of surinamite. As for the sapphirine refinement

Table 7. Surinamite: electrostatic valence balance of cations and anions†

	M(1) 2/6	M(2) 3/6	M(3) 3/6	M(4) 3/6	M(5) 2/6	M(6) 3/6	M(7) 2/6	M(8) 2/6	M(9) 3/6	T(1) 2/4	T(2) 4/4	T(3) 4/4	T(4) 4/4	T(5) 3/4	Δp_0
O(1)	------	------	-0.028	------	-0.044	------	------	------	------	------	-0.014	------	------	------	-0.167
O(2)	------	------	-0.051	------	------	------	------	-0.016	------	------	------	------	-0.012	------	-0.167
O(3)	------	------	+0.022	------	------	------	+0.010	+0.025	------	------	+0.022	------	------	------	+0.167
O(4)	------	------	+0.001	+0.044	+0.089	------	------	------	------	------	------	------	+0.017	-----	+0.333
O(5)	------	------	------	------	------	------	------	-0.008	------	------	+0.008	------	------	-0.009	+0.083
O(6)	------	------	------	------	-0.045	------	------	------	------	-0.003	------	------	-0.021	------	-0.167
O(7)	----	-0.066	+0.003	------	------	------	-0.028	------	------	+0.007	------	------	------	------	-0.167
O(8)	-0.045	------	------	------	------	------	------	------	------	------	------	------	+0.016	+0.000	+0.083
O(9)	------	+0.001	+0.051	-0.073	------	------	------	------	------	------	------	------	------	-0.003	+0.250
O(10)	-0.106	------	------	------	------	------	------	------	------	-0.009	-0.015	------	------	------	-0.167
O(11)	-0.153	------	------	------	------	------	------	------	------	+0.004	------	-0.033	------	------	-0.167
O(12)	------	-0.088	------	+0.030	------	------	------	------	------	------	------	-0.021	------	------	+0.000
O(13)	+0.037	------	------	------	------	-0.017	------	------	+0.018	------	------	------	------	+0.010	+0.083
O(14)	------	-0.049	------	------	------	-0.042	+0.017	------	-0.052	------	------	------	------	------	-0.167
O(15)	+0.160	+0.057	------	------	------	+0.059	------	------	------	------	------	+0.023	------	------	+0.333
O(16)	+0.105	+0.144	------	------	------	------	------	------	+0.033	------	------	+0.032	------	------	+0.333

†A bond length deviation refers to the polyhedral average subtracted from the individual bond distance. The Δp_0 = deviations of electrostatic bond strength sum from neutrality (p_0 = 2.00 e.s.u.). Bond length deviations which conform to Δp_0 are underlined.

of Moore (1969), the bond distances have been arranged according to increasing bond length. Distortion of the polyhedra is complex, like sapphirine, because not only shared edges but also a range of cationic sizes, charges and substitutions occurs. There is a pronounced tendency, however, for shared edge distances to appear at the top of the list of distances for a polyhedron in Table 6 since the distances were listed according to increasing values.

Finally, a tabulation of electrostatic valence balances appears in Table 7. Since all the principal ions have inert gas configurations, an electrostatic model is sensible. Of the 56 entries in the table, 44 are in conformity with expected bond length–bond strength deviations, or 79% of the admissible data. The 12 contradictions generally show small deviations of individual bond distance from the polyhedral average. One problem remains in ascribing the correct bond strengths for the individual polyhedra since the site populations, especially between Mg^{2+} and Al^{3+}, are not accurately known.

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