

GITTINSITE: A MODIFICATION OF THE THORTVEITITE STRUCTURE

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ABSTRACT

Gittinsite ($\text{CaZrSi}_2\text{O}_7$) is monoclinic, with space group $C2$ and a 6.852(2), b 8.659(1), c 4.686(2) Å, β 101.69(2)° and $Z = 2$. The crystal structure of gittinsite is a modification of the thortveitite (Sc_2SiO_7) structure. Both structures contain isolated Si_2O_7 groups. In gittinsite, the edge-sharing calcium-oxygen and zirconium-oxygen octahedra form sheets parallel to the (001) plane, which are connected by Si_2O_7 groups located above and below a void centered at 0.5, 0.5, 0.5. Differences between the gittinsite and thortveitite (a 6.452, b 8.519, c 4.669 Å and β 102.55°) structures are a result of the replacement of the two Sc^{3+} atoms in thortveitite by the Ca^{2+} and Zr^{4+} atoms in gittinsite. In thortveitite ($C2/m$), the scandium sites are equivalent, and the Si-O-Si angle is required to be 180°, whereas in gittinsite ($C2$), the bridging angle is 147.4(5)°. Comparison of the Si_2O_7 unit of gittinsite with Si_2O_7 units in other structures reveals bond lengths and angles equal within experimental errors to the mean of 27 other Si_2O_7 groups.

Keywords: gittinsite, structure determination, calcium zirconium silicate, Si_2O_7 , X-ray diffraction, thortveitite, Strange Lake alkaline complex, Quebec, Labrador.

SOMMAIRE

La gittinsite $\text{CaZrSi}_2\text{O}_7$ est monoclinique (groupe spatial $C2$), et possède les paramètres réticulaires a 6.852(2), b 8.659(1), c 4.686(2) Å, β 101.69(2)° pour $Z = 2$. Sa structure cristalline est une modification de celle de la thortveitite $\text{Sc}_2\text{Si}_2\text{O}_7$. Les deux structures contiennent des groupes Si_2O_7 isolés. Dans la gittinsite, les octaèdres Ca-O et Zr-O, à arêtes partagées, forment des feuillets parallèles à (001) qui sont liés par les groupes Si_2O_7 situés par dessus et au dessous d'une cavité centrée sur 0.5, 0.5, 0.5. Les différences entre la thortveitite (a 6.452, b 8.519, c 4.669 Å, β 102.55°) et la gittinsite découlent du remplacement de deux atomes de Sc^{3+} par Ca^{2+} et Zr^{4+} . Dans la thortveitite ($C2/m$), les deux atomes de scandium occupent une seule position, et l'angle Si-O-Si doit être égal à 180°, tandis que dans la gittinsite, l'angle équivalent est 147.4(5)°. Les longueurs de liaisons et les angles du groupe Si_2O_7 de la gittinsite sont les mêmes, aux erreurs expérimentales près, que dans 27 autres structures.

(Traduit par la Rédaction)

Mots-clés: gittinsite, affinement de la structure, silicate de calcium et de zirconium, Si_2O_7 , diffraction X, thortveitite, complexe alcalin de Strange Lake, Québec, Labrador.

INTRODUCTION

Gittinsite ($\text{CaZrSi}_2\text{O}_7$) was first reported as an unidentified calcium zirconium silicate by Gittins *et al.* (1973) in pegmatitic lenses and gneisses of gabbroic peralkaline rocks at Kipawa River, Villedieu Township, Temiscaming County, Quebec. Ansell *et al.* (1980) named the new calcium zirconium silicate *gittinsite* and described its optical and physical properties. Electron-microprobe analysis of gittinsite gave CaO 18.4%, ZrO₂ 40.3% and SiO₂ 40.8% for a total of 99.5% (Plant & Roberts 1979), producing an empirical formula of $\text{CaZrSi}_2\text{O}_7$ based on seven oxygen atoms. The unit-cell dimensions and β angle were determined through the use of X-ray powder diffraction by Plant & Roberts (1979) and Ansell *et al.* (1980). They also noticed the similarities between the gittinsite and the thortveitite powder patterns. The material that is the subject of this investigation occurs in the Strange Lake alkaline complex. The complex is located on the Quebec-Labrador border, 250 km northeast of Schefferville and 150 km west of Nain (on the Labrador coast), just southeast of Lac Brisson (Miller 1986). The aegirine-riebeckite-bearing peralkaline granite is subdivided into three major phases; exotic-poor, exotic, and exotic-rich (Miller 1988). The phases are characterized by decreasing age and increasing exotic-mineral and rare-metal content. The exotic minerals include: elpidite $\text{Na}_2\text{ZrSi}_6\text{O}_{15} \cdot 3\text{H}_2\text{O}$, pyrochlore, armstrongite $\text{CaZrSi}_6\text{O}_{15} \cdot 2.5\text{H}_2\text{O}$, gittinsite, gadolinite-(Y) $\text{Y}_2\text{Fe}^{2+}\text{Be}_2\text{Si}_2\text{O}_{10}$, kainosite $\text{Ca}_2(\text{Ce}, \text{Y})_2\text{Si}_4\text{O}_{12}(\text{CO}_3) \cdot \text{H}_2\text{O}$, allanite, thorite and titanite, plus rare metals and several unnamed minerals (Miller 1986, 1988). Gittinsite accompanied by aegirine and iron oxides isomorphously replaces elpidite at Strange Lake (Currie 1985).

CRYSTAL DATA

The specimen of gittinsite (NMC 66057) studied was obtained from Dr. J. Jambor of CANMET, Ottawa. The small colorless tabular ($0.08 \times 0.13 \times 0.10$ mm) crystal was mounted on a CAD4 computer-controlled single-crystal X-ray diffractometer. The unit-cell dimensions were determined by least-squares refinement of the 2θ values measured from 25 reflections, using graphite-monochromated $\text{MoK}\alpha$ radi-

TABLE 1. GITTINSITE STRUCTURE-REFINEMENT DATA

Ideal formula:	CaZrSi ₂ O ₇	Radiation:	MoK α , graphite monochromated (45 kV, 16 ma)
Space Group:	C2	No. of I ₀ measured:	1886
a(Å):	6.852(2)	No. of 1>3.0 σ (I) ¹ :	1027
b(Å):	8.659(1)	No. of reflections:	513
c(Å):	4.686(2)	Final R:	3.1%
β (°):	101.69(2)	Final R _w :	3.9%
V(Å ³):	272.1(1)		
Z:	2		

¹ $\sigma(I)$ is the standard deviation of the intensity (I) as determined from counting statistics.

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

$$R_w = \frac{[\sum (F_o - F_c)^2 / w]}{\sum F_o^2}$$

$$w = 1/(\text{SIGF})^2 = 4^* \text{FSQ}/\text{SIGFSQ}^2$$

$$\text{SIGFSQ} = \text{SQRT}[\text{SIG1}^2 + (P^* \text{FSQ})^2]$$

$$\text{SIGF} = \text{SIGFSQ}/(2^*F)$$

F - observed structure factor amplitude

FSQ - F²

SIGF - standard deviation on F

SIGFSQ - standard deviation on F squared

SIG1 - standard deviation on I, based on counting statistics

P - experimental instability factor used to downweight the intense reflections = 0.04

w - weight for the reflection

TABLE 2. ATOMIC PARAMETERS AND TEMPERATURE-FACTOR COEFFICIENTS FOR GITTINSITE

	Zr	Ca	Si	O ₁	O ₂	O ₃	O ₄
x	0.0000	0.0000	0.2123(2)	0.0000	0.3734(6)	0.1885(8)	0.2640(7)
y	0.3140(2)	0.7063(2)	0.9920(2)	0.9387(9)	0.0000	0.1549(6)	0.8539(5)
z	0.5000	0.5000	0.9187(4)	0.0000	0.2196(10)	0.7405(11)	0.7103(0)
B_{iso} (Å ²)	0.74(1)	1.36(4)	0.83(3)	1.61(16)	1.06(9)	1.42(11)	1.08(12)
U ₁₁	0.0103(2)	0.0179(9)	0.0128(7)	0.013(2)	0.016(2)	0.030(2)	0.021(2)
U ₂₂	0.0099(4)	0.0104(8)	0.0126(8)	0.029(4)	0.016(2)	0.012(2)	0.016(4)
U ₃₃	0.0096(3)	0.027(1)	0.0086(7)	0.027(4)	0.012(2)	0.015(2)	0.013(2)
U ₁₂	0.0000	0.0000	0.002(1)	0.0000	0.001(3)	0.001(6)	-0.004(3)
U ₁₃	0.0015(5)	-0.014(2)	-0.001(1)	0.007(6)	-0.008(3)	-0.006(5)	0.005(5)
U ₂₃	0.0000	0.0000	-0.001(2)	0.0000	0.002(6)	0.001(4)	-0.009(4)

$$U_{11} = \beta_{11} 2a^2 a^2$$

$$U_{22} = \beta_{22} 2a^2 b^2$$

$$U_{33} = \beta_{33} 2a^2 c^2$$

$$U_{12} = \beta_{12} 2a^2 a^2 b^2$$

$$U_{13} = \beta_{13} 2a^2 a^2 c^2$$

$$U_{23} = \beta_{23} 2a^2 b^2 c^2$$

tion. These values are in good agreement with those determined by Ansell *et al.* (1980) and Plant & Roberts (1979). The operating conditions and the resulting unit cell dimensions are listed in Table 1.

COLLECTION OF INTENSITY DATA

X-ray intensity data were collected on the diffractometer from the crystal described above. No tests of centrosymmetry were performed. The rate of the θ - 2θ scans was varied in order to obtain a σ_1/I of 0.02 where possible within a 60-second counting period. Three standard reflections were measured every two hours. Their intensity did not vary by more than 1% during the data collection. A hemisphere with $\pm h \pm k \pm l$ reflections with theta less than 30° was measured. A summary of the data collection is presented in Table 1. No corrections for absorption or extinction were applied.

DETERMINATION AND REFINEMENT OF THE STRUCTURE

Cruickshank *et al.* (1962) considered the likelihood of space groups $C2/m$, $C2$, and Cm for thortveitite. The space group Cm was rejected owing to the impossible bond-lengths produced in the Si₂O₇ groups, and $C2$ as well, owing to discrepancies in the O-Si-O angles. Therefore, $C2/m$ was accepted as the space group for thortveitite.

Given the observed diffraction-symmetry and systematic absences, the possible space-groups for gittinsite are $C2/m$, $C2$ and Cm . Owing to similarities between the gittinsite and thortveitite structures, the coordinates of thortveitite (Cruickshank *et al.* 1962) were used as starting parameters in the least-squares refinement. However, in the thortveitite structure, the scandium atoms occupy only one symmetrically unique octahedral position. In gittinsite, which contains both calcium and zirconium atoms, the octahedral site must be disordered with respect to occupancy (space groups $C2/m$ and Cm), or the symmetry must be lowered to $C2$. Space group $C2$ was chosen based on the realistic bond-lengths and angles produced, and the least-squares site-occupancy refinement of the octahedral position.

Structure refinement was performed with the use of the structure determination package of Frenz *et al.* (1983). Refinement with isotropic temperature-factors, using the atomic positions for $C2$ as listed in Cruickshank *et al.* (1962), resulted in convergence with an unweighted R factor of 4.8%. With anisotropic temperature-factors, the final unweighted R factor dropped to 3.1% and the weighted R factor to 3.9%. No disorder was observed between the calcium and zirconium cations in the two nonequivalent octahedral sites. The final atomic parameters and temperature-factor coefficients for gittinsite are listed in Table 2.

Observed and calculated structure-factors have been submitted to the Depository of Unpublished Data, CISTI, National Research Council of Canada, Ottawa, Canada K1A 0S2.

DISCUSSION OF THE STRUCTURE

The crystal structure of gittinsite consists of octahedral sheets that are one third filled with calcium, one third filled with zirconium and one third vacant. The sheets are separated by Si₂O₇ groups, producing a void in the center of the unit cell (Fig. 1). The calcium-oxygen octahedra share three edges with the zirconium-oxygen octahedra and three edges with the octahedral voids to form the octahedral layer. Likewise, the octahedral voids share three edges with zirconium-oxygen octahedra. These voids show an irregular octahedral coordination, with a quadratic elongation of 1.136(4). The six shorter oxygen-void

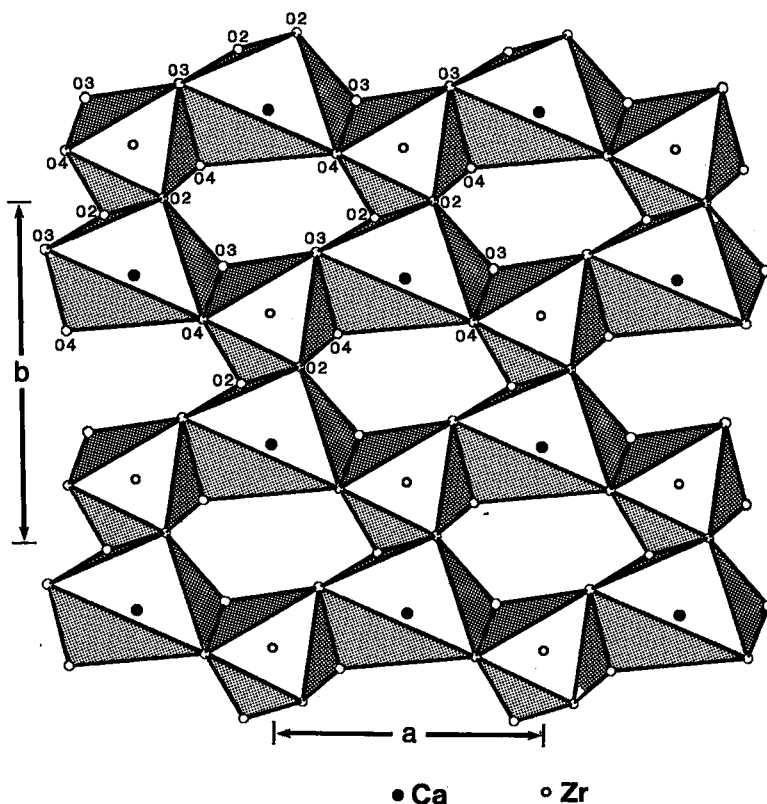


FIG. 1. A (001) projection of the layer of octahedra in gittinsite. All diagrams were produced using ORTEP (Johnson 1965).

center distances average 2.232 \AA , and the two longer oxygen-void center distances are 3.109 \AA . The unoccupied site is octahedrally coordinated (Fig. 2) and has a polyhedral volume of $12.4(1) \text{ \AA}^3$.

The geometry of the different octahedra is compared in Table 3. Both calcium and zirconium form distorted octahedra with the surrounding oxygen atoms. The distortions of the calcium and zirconium octahedra are caused by shortening of the shared octahedral edges. Each octahedron shares one O_2-O_2 edge as well as two O_3-O_4 edges with other octahedra. In the octahedra, the mean calcium-oxygen distance is $2.397(8) \text{ \AA}$, whereas the mean zirconium-oxygen distance is $2.100(8) \text{ \AA}$.

The CaO_6 octahedra in gittinsite show greater deformation than either the ZrO_6 octahedra in gittinsite or the ScO_6 octahedra in thortveitite. This deformation can be observed directly in Figure 1 and through examination of the quadratic elongations in Table 3. The ZrO_6 octahedra in gittinsite are more regular than to the ScO_6 octahedra in thortveitite, although the polyhedral volume remains equal (Table 3).

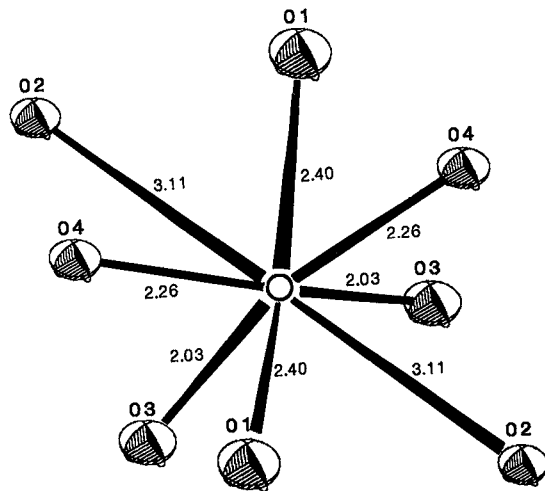


FIG. 2. Atoms surrounding the void in gittinsite. Note the six similar distances and the two longer distances. The void is located at 0.5, 0.5, 0.5. Distances are in \AA .

TABLE 3. OCTAHEDRA: DISTANCES AND ANGLES

BOND LENGTHS (ANGSTROMS)					
Gittinsite			Thortveitite*		
Ca	Zr		Sc		
Ca-O ₂	2.275(5) x2	Zr-O ₂	2.151(5) x2	Sc-O ₂	2.12 x2
Ca-O ₃	2.646(5) x2	Zr-O ₃	2.063(5) x2	Sc-O ₃	2.09 x2
Ca-O ₄	2.270(4) x2	Zr-O ₄	2.085(4) x2		2.20 x2
Mean	2.397(8)	Mean	2.100(8)	Mean	2.13
0 ₂ -O ₂	2.840(8) ^f	0 ₂ -O ₂	2.840(8) ^f	0 ₂ -O ₂	2.68 ^f
0 ₂ -O ₃	3.256(7) x2	0 ₂ -O ₃	3.038(6) x2	0 ₂ -O ₃	2.75 x2
	3.253(6) x2		2.752(6) x2		3.02 x2
0 ₂ -O ₄	3.235(7) x2	0 ₂ -O ₄	2.858(6) x2		3.07 x2
			3.065(9)	0 ₃ -O ₃	2.59 x2 ^f
0 ₃ -O ₄	2.796(6) x2 ^f	0 ₃ -O ₄	2.796(6) x2 ^f		3.28
	4.331(6) x2		3.360(6) x2		3.63 x2
0 ₄ -O ₄	3.753(9)				
Quadratic ²		Quadratic ²		Quadratic ²	
Elongation	1.111(3)	Elongation	1.026(2)	Elongation	1.061
Volume(Å ³)	15.9(2)	Volume(Å ³)	11.9(1)	Volume(Å ³)	11.9
BOND ANGLES (DEGREES)					
0 ₂ -Ca-O ₂	77.2(2)	0 ₂ -Zr-O ₂	82.6(2)	0 ₂ -Sc-O ₂	78.7
0 ₂ -Ca-O ₃	82.5(2) x2	0 ₂ -Zr-O ₃	92.2(2) x2	0 ₂ -Sc-O ₃	79.0 x2
	82.4(2) x2		81.0(2) x2		88.9 x2
0 ₂ -Ca-O ₄	90.7(2) x2	0 ₂ -Zr-O ₄	84.8(2) x2		93.8 x2
			95.0(3)	0 ₃ -Sc-O ₃	74.3 x2
0 ₃ -Ca-O ₄	68.8(1) x2	0 ₃ -Zr-O ₃	84.7(2) x2		103.8
	123.4(1) x2	0 ₃ -Zr-O ₄	108.1(2) x2		115.9 x2
0 ₄ -Ca-O ₄	111.5(2)				

* Atomic positions from Cruickshank *et al.* (1962)^f Shared edges² From Hazen & Finger (1982)

TABLE 4. TETRAHEDRA: DISTANCES AND ANGLES

BOND LENGTHS (ANGSTROMS)			
Gittinsite		Thortveitite*	
Si-O ₁	1.643(2)	Si-O ₁	1.60
Si-O ₂	1.607(4)	Si-O ₂	1.62
Si-O ₃	1.630(5)	Si-O ₃	1.63 x2
Si-O ₄	1.628(4)		
Mean	1.627(8)	Mean	1.62
0 ₁ -O ₂	2.613(4)	0 ₁ -O ₂	2.54
0 ₁ -O ₃	2.698(7)	0 ₁ -O ₃	2.61 x2
0 ₁ -O ₄	2.578(5)		
0 ₂ -O ₃	2.696(6)	0 ₂ -O ₃	2.72 x2
0 ₂ -O ₄	2.675(6)		
0 ₃ -O ₄	2.667(6)	0 ₃ -O ₄	2.67
Quadratic ^f		Quadratic ^f	
Elongation	1.003(5)	Elongation	1.004
Volume(Å ³)	2.19(3)	Volume(Å ³)	2.2
BOND ANGLES (DEGREES)			
Si-O ₁ -Si	147.4(5)	Si-O ₁ -Si	180.0
0 ₁ -Si-O ₂	107.1(2)	0 ₁ -Si-O ₂	104.1
0 ₁ -Si-O ₃	111.1(3)	0 ₁ -Si-O ₃	107.7 x2
0 ₁ -Si-O ₄	104.1(3)		
0 ₂ -Si-O ₃	112.8(3)	0 ₂ -Si-O ₃	113.4 x2
0 ₂ -Si-O ₄	111.6(3)		
0 ₃ -Si-O ₄	109.9(2)	0 ₃ -Si-O ₄	110.1
Mean	109.1	Mean	109.4

* Atomic positions from Cruickshank *et al.* (1962)^f From Hazen & Finger (1982)

The Si₂O₇ groups consist of two corner-sharing SiO₄ tetrahedra (Fig. 3a). The silicon atoms share O₁, whereas the rest of the oxygen atoms in each tetrahedron are bonded to the silicon atom, as well

as a calcium and a zirconium atom. The tetrahedra are rotated by approximately 180° with respect to each other about the Si-O-Si linkage. The tetrahedra show little deformation in either gittinsite or thortveitite (Table 4). Each Si₂O₇ group is bonded by the

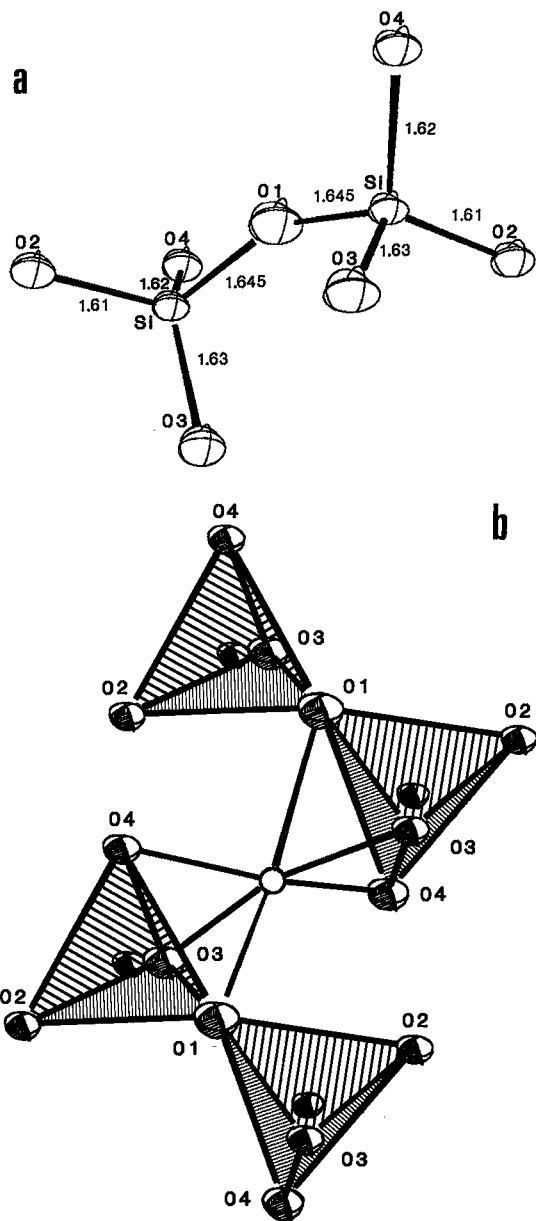


FIG. 3. a) The Si₂O₇ group in gittinsite. Distances are in Å. b) The void in gittinsite surrounded by the Si₂O₇ groups. The thermal ellipsoids represent 65% probability distribution in both figures.

TABLE 5. BOND LENGTHS AND ANGLES OF Si_2O_7 GROUPS IN SILICATES

	$d(\text{Si}-\text{O}(\text{nonbr}))\text{\AA}$	$d(\text{Si}-\text{O}(\text{br}))\text{\AA}$	$\Delta\text{Si}-\text{O}-\text{Si}^\circ$
Mean values*	1.619	1.644	148.2
Gittinsite	1.622(8)	1.643(2)	147.4(5)
	$\angle\text{O}(\text{nonbr})-\text{Si}-\text{O}(\text{nonbr})^\circ$	$\angle\text{O}(\text{br})-\text{Si}-\text{O}(\text{nonbr})^\circ$	$\Delta\text{d}\text{\AA}$
Mean values*	111.7	107.1	0.025
Gittinsite	111.4(5)	107.4(5)	0.021(8)

Note: $\Delta\text{d} = d(\text{Si}-\text{O}(\text{bridging})) - d(\text{Si}-\text{O}(\text{nonbridging}))$

* Liebau (1985) for 27 silicates containing Si_2O_7 groups.

oxygen atoms at the intersection of the octahedra to the layers of CaO_6 and ZrO_6 octahedra. One corner of a silicate tetrahedron is shared by the lower layer of octahedra, whereas the two top corners are shared by the upper layer. The other silicate tetrahedron shares one corner with the upper octahedral layer and two corners with the lower layer. The voids are located between two Si_2O_7 groups, forming chains parallel to c of alternating Si_2O_7 groups and voids (Fig. 3b).

The mean $\text{Si}-\text{O}_{\text{nonbr}}$ bond length in the Si_2O_7 group is 1.622(8) Å (Table 4). The value of the bond lengths of the two $\text{Si}-\text{O}_{\text{br}}$ (or $\text{Si}-\text{O}_1$) bonds of the Si_2O_7 group is 1.643(2) Å. The mean value of the six $\text{O}_{\text{nonbr}}-\text{Si}-\text{O}_{\text{nonbr}}$ angles of the Si_2O_7 group is 111.4(5)°. The mean value of the six $\text{O}_{\text{br}}-\text{Si}-\text{O}_{\text{nonbr}}$ angles of the Si_2O_7 group is 107.4(9)°, and the angle $\text{Si}-\text{O}_1-\text{Si}$ is 147.4(5)°. Comparison of these values with other Si_2O_7 groups (Liebau 1985) shows that the dimensions of the Si_2O_7 group in gittinsite are approximately equal to the average dimensions of the Si_2O_7 groups in other minerals (Table 5). Cation repulsion between the two silicon atoms in the $\text{Si}-\text{O}_{\text{br}}-\text{Si}$ arrangement produces a $\text{Si}-\text{O}_{\text{br}}$ bond length greater than the mean $\text{Si}-\text{O}_{\text{nonbr}}$ bonds and a mean $\text{O}_{\text{nonbr}}-\text{Si}-\text{O}_{\text{nonbr}}$ angle greater than the $\text{O}_{\text{br}}-\text{Si}-\text{O}_{\text{nonbr}}$ angle. Repulsion between the two silicon atoms through the bridging oxygen atom causes the silicon atoms to be displaced from the center of the silicate tetrahedra.

The gittinsite structure represents a variant of the thortveitite structure. The silicon atom, which is at $(x, 0, z)$ in thortveitite, is moved to a general position in gittinsite. The O_1 atoms lie in general positions in gittinsite, but in thortveitite they lie on the center of symmetry. The octahedrally coordinated scandium cations in thortveitite ($C2/m$) are crystallographically equivalent. In gittinsite, differences between the octahedrally coordinated calcium and zirconium require two different cation sites, thereby reducing the space group to $C2$.

CONCLUSIONS

The octahedral layer is composed of edge-sharing

octahedra. One third of the octahedra contain calcium, one third zirconium, and one third unfilled octahedral voids. The Si_2O_7 groups, which link the octahedral sheets, are located above and below each void. The structure of gittinsite can be considered a modification of the thortveitite structure in which the space group is lowered to $C2$ from $C2/m$. The bond lengths and angles in the Si_2O_7 group of gittinsite are equal to the mean for the 27 silicates containing Si_2O_7 groups, as compiled by Liebau (1985).

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