THE CRYSTAL STRUCTURE OF GERENITE-(Y), \((\text{Ca}, \text{Na})_2(Y, \text{REE})_3\text{Si}_6\text{O}_{18}\cdot2\text{H}_2\text{O}\),
A CYCLOSILICATE MINERAL

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ABSTRACT

The crystal structure of gerenite-(Y), ideally \((\text{Ca}, \text{Na})_2(Y, \text{REE})_3\text{Si}_6\text{O}_{18}\cdot2\text{H}_2\text{O}\), \(a = 9.257(4), b = 9.684(4), c = 5.520(1)\, \AA\), \(\alpha = 97.36(3), \beta = 100.52(3), \gamma = 116.57(3)^\circ\), \(V = 422.6(3)\, \AA^3\), space group \(P\overline{1}\), \(Z = 1\), has been solved by direct methods, and refined to an \(R\) index of 5.2\% based on 2175 unique reflections measured with \(\text{MoK}_\alpha\) radiation. The structure consists of the following elements: (1) \(\text{Si}_6\text{O}_{18}\) rings, oriented approximately parallel to \((-101)\), (2) chains of edge-sharing \(\text{Y}(1)\text{O}_6\) and \(\text{Y}(2)\text{O}_6\) octahedra oriented approximately parallel to \([101]\), and (3) \(\text{CaO}_6\) polyhedra. The \(\text{Si}_6\text{O}_{18}\) rings share corners with the chains of \(\text{YO}_6\) octahedra to form a three-dimensional framework. The \(\text{Ca}\) positions are located outside of and between pairs of \(\text{Si}_6\text{O}_{18}\) rings. Bond-valence analysis shows that one of the apical anions coordinating the cation at the \(\text{Ca}\) position is a molecule of \(\text{H}_2\text{O}\). The \(\text{CaO}_6\) polyhedra share corners and edges with adjacent \(\text{Si}_6\text{O}_{18}\) rings and \(\text{YO}_6\) chains. The crystal structure of gerenite-(Y) has elements similar to those of kainosite-(Y) and leifite, both of which occur with gerenite-(Y) at the Strange Lake locality.

Keywords: gerenite-(Y), crystal structure, cyclosilicate, Strange Lake, Quebec - Labrador.

INTRODUCTION

As described in Jambor et al. (1998), gerenite-(Y) occurs in the Strange Lake peralkaline granitic complex, about 250 km northeast of Schefferville, on the Quebec - Labrador border. The intrusive complex contains a deposit of \(Y\), the rare-earth elements \((\text{REE})\), \(\text{Nb}, \text{Zr}\), and \(\text{Be}\), mostly within a thick lens of pegmatite and aplite. In addition to gerenite-(Y), the pegmatite - aplite lens contains quartz, albite, K-feldspar, aegirine, riebeckite - arvedsonite, gittinsite, zircon and kainosite-(Y), and small amounts of pyrochlore, thorite, a new gadolinite-type mineral, titania, fluoride, epidote, hematite, monazite-(Ce), and sphalerite (Miller 1996, Jambor et al. 1998).

Most gerenite-(Y) occurs in the pegmatite - aplite lens at anhedral masses composed of an intergrowth of gerenite-(Y), kainosite-(Y), and quartz. The gerenite-(Y) typically forms bundles \((100 \times 20 \, \mu\text{m})\) of slightly divergent elongate grains with interstitial quartz. According to Miller (1996), the anhedral masses may be pseudomorphic after leifite. Gerenite-(Y) also occurs in the pegmatite - aplite lens as elongate, prismatic grains of primary origin.

Using precession photographs of a crystal from an intergrowth, Jambor et al. (1998) concluded that...
gerenate-(Y) is triclinic (space group P1 or P1'). The unit-cell parameters (refined from powder data) are $a = 9.245(5)$, $b = 9.684(6)$, $c = 5.510(3)$ Å, $\alpha = 97.44(6)$, $\beta = 100.52(6)$, $\gamma = 116.70(6)^{\circ}$, $V = 420.8(1)$ Å³. The average chemical composition (based on results of three electron-microprobe analyses by D.R. Owens) is (in wt.%): Na₂O 1.7, CaO 7.6, MnO 0.6, Y₂O₃ 28.2, Ce₂O₃ 0.1, Nd₂O₃ 0.2, Sm₂O₃ 0.3, Gd₂O₃ 1.1, Tb₂O₃ (estimated from chondrite-normalized REE spectra) 0.34, Dy₂O₃ 4.0, Ho₂O₃ (estimated) 1.05, Er₂O₃ 3.6, Tm₂O₃ (estimated) 0.51, Yb₂O₃ 2.9, Lu₂O₃ (estimated) 0.41, SiO₂ 40.5, H₂O (by difference) 6.89, total 100.0. Recalculation on the basis of 18 O atoms gave (in wt.%) Na 0.49, Ca 1.21, Y 2.24, REE (estimated from chondrite-normalized REE spectra) 0.41, SiO₂ 40.5, H₂O (by difference) 5.89, total 100.0. This study was undertaken to determine the crystal structure of gerenate-(Y) and to study the role of H₂O in the structure.

**EXPERIMENTAL.**

The crystal used in this study was of the prismatic (primary) type, obtained (as a plate) from a thin section. The bounding face was a polished surface with approximate index (011). The crystal was mounted on a Siemens P3 automated four-circle diffractometer equipped with a molybdenum-target X-ray tube (operating at 50 kV, 35 mA) and a precisely oriented graphite crystal monochromator mounted with equatorial geometry. Forty-two reflections with $15.06 < 2\theta < 32.56^\circ$ were centered using an automated search routine, and the correct unit-cell was selected from an array of real-space vectors corresponding to potential unit-cell axes. Least-squares refinement of these reflections produced the cell dimensions given in Table 1, together with the orientation matrix relating reflections produced the cell dimensions given in Table 1. The crystal was modeled as a thin plate with approximate index (2 11 11). A minimum glancing angle of $5^\circ$ resulted in the loss of 38 reflections. The merging $R$ index for the $\psi$-scan data set decreased from 6.9% before the absorption correction to 4.2% after the absorption correction. This correction was then applied to the entire dataset; minimum and maximum transmissions were 0.368 and 0.588, respectively. The data were also corrected for Lorentz, polarization and background effects, averaged and reduced to structure factors. Of the 2175 unique reflections, 1369 were classed as observed ($I > 3\sigma(I)$).

**Structure Solution and Refinement.**

The Siemens SHELXTL PC system of programs was used throughout this study. Scattering curves for neutral atoms together with anomalous dispersion coefficients were taken from Cromer & Mann (1968) and Cromer & Liberman (1970). The scattering curve for H₂O was used to represent the rare-earth elements (REE) on the basis of the weighted average of the atomic numbers, calculated from the average results of the electron-microprobe analyses in Jambor et al. (1998). Miscellaneous information on data collection and refinement is given in Table 1.

| $a$ (Å) | 9.257(4) | $Z$ | 1 |
| $b$ | 9.864(4) | Crystal size (mm) | 0.1 x 0.1 x 0.01 |
| $c$ | 5.520(1) | $\mu$(MoKα, mm⁻¹) | 12.10 |
| $\alpha$ (°) | 97.44(6) | Red/mono | MoKα/graphite |
| $\beta$ | 100.52(3) | Total R | 2175 |
| $\gamma$ | 116.70(6) | $R$ | 5.2 |

**TABLE 1. MISCELLANEOUS INFORMATION: GERENITE-(Y)**

| $F_0$ | $F_{oxygen}$ | $R$ (%) | 6.8 |

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

$wR = \frac{\sum [w(F_o - F_c)^2]^{1/2}}{\sum w F_o^2}$, $w = [\sigma^2 F + 0.00487 F^2]^{-1}$

A mean $[E^2 - 1]$ value of 0.89 implies a centrosymmetric space-group. Systematic absences in the complete data-set suggested space group $P1$. The structure was solved by direct methods and refined in $P1$ to an $R$ index of 9.9% for an isotropic displacement model. Further refinement was done using anisotropic displacement factors for all atoms in the structure. Assuming full occupancy for all sites (and refining Ca:Na and Y:REE for the Ca and Y sites, respectively) led to convergence at $R$ and $wR$ indices of 5.1 and 5.2%, respectively. However, the results show excess positive charge at the Ca position, as the Ca:Na ratio is 1:0.56, and the bond-valence sum to the Ca position is 1.87. These values must be 1:1 and 1.5, respectively, if the Y sites are fully occupied by trivalent cations, and the H₂O site is fully occupied by H₂O (as indicated by the bond-valence value of 0.33 valence units). The results suggest that there are vacancies at the Ca and
Y sites. Additional refinements were done with the occupancies fixed at the values given by the electron- 
microprobe results (including estimated elements). This 
resulted in final $R$ and $wR$ values of 5.2 and 6.8%, 
respectively (8.8 and 9.4% for all 2175 data). Addition 
of an isotropic extinction correction did not improve 
the results. The program MISSYM (Le Page 1987) was 
used to search for additional elements of symmetry; 
none was indicated. Positional coordinates and 
anisotropic and equivalent isotropic-displacement 
factors are given in Table 2. Interatomic distances and 
angles are given in Table 3, and a bond-valence 
analysis in Table 4. Structure factors may be obtained 
from the Depository of Unpublished Data, CISTI, 
National Research Council, Ottawa, Ontario K1A 0S2.

DESCRIPTION OF THE STRUCTURE

There are six distinct cation sites in the gerenite-(Y) 
structure. Three of the cation sites are occupied by Si. 
The Si(1)–O distances range from 1.580 to 1.623 Å 
(mean 1.606 Å), and the O–Si(1)–O angles, from 104.2 
to 116.1° (mean 109.4°). The Si(2)–O distances 
 vary from 1.600 to 1.632 Å (mean 1.616 Å), and 
the O–Si(2)–O angles, from 105.4 to 117.1° (mean 
109.3°). The Si(3)–O distances range from 1.591 
to 1.644 Å (mean 1.616 Å), and the O–Si(3)–O angles, 
from 104.8 to 115.7° (mean 109.4°). The Si(1) 
tetrahedron is somewhat smaller than the Si(2) and 
Si(3) tetrahedra; the polyhedral volumes are 2.11 
and 2.15 (× 2) Å$^3$, respectively. The SiO$_4$ tetrahedra share corners to form [Si$_6$O$_{18}$]$^{12-}$ 
rings oriented approximately parallel to (101) (Figs. 1, 
2). The bridging O atoms are O(4), O(8) and O(9). In 
general, the bonds to the bridging O atoms are longer 
than those to the non-bridging O atoms (Table 2). The 
Si(1)–Si(2) and Si(1)–Si(3) distances are similar 
(3.211 and 3.225 Å, as are the Si(1)–O(9)–Si(2) and 
Si(1)–O(8)–Si(3) angles (167.1 and 167.3°). The 
Si(2)–Si(3) distance is somewhat shorter (3.108 Å, 
and the Si(2)–O(4)–Si(3) angle is more acute (145.8°). 

The atom at the Y(1) site, at special position $1e$ 
($\frac{1}{2}, \frac{1}{2}, 0$), is coordinated by six O atoms, forming a 
distorted octahedron. The Y(1)–O distances are 2.207, 
2.300, and 2.315 Å (all × 2; mean 2.274 Å), and the 
O–Y(1)–O angles range from 72.8 to 107.2° (mean 
90.0°). The mean quadratic elongation of the octahedra 
(Robinson et al. 1971) is 1.033, and the polyhedron's 
volume is 14.95 Å$^3$. The atom at the Y(2) site is coordinated by six O atoms, forming a 
distorted octahedron. The Y(2)–O distances range from 2.220 to 2.326 Å (mean 2.279 Å), and the 
O–Y(2)–O angles range from 73.7 to 106.5° (mean 90.5°). The mean quadratic elongation of the octahedra 
is 1.033, and the polyhedron's volume is 15.03 Å$^3$. The Y(1) and Y(2) octahedra share edges to form 
chains with the repeat pattern Y(1), Y(2), Y(2)... The 
chains of octahedra run approximately parallel to 
[101]. Each Y(1) octahedron shares two O(3)–O(5) 
edges with two Y(2) octahedra. The two shared edges 
are considerably shorter (2.74 Å) than the distance between O(4) and O(8) pairs (5.23 and 5.27 Å, respectively). 

The Y(1) and Y(2) octahedra share edges to form 
chains with the repeat pattern Y(1), Y(2), Y(2)... The 
chains of octahedra run approximately parallel to 
[101]. Each Y(1) octahedron shares two O(3)–O(5) 
edges with two Y(2) octahedra. The two shared edges 
are considerably shorter (2.74 Å) than the ten unshared 

<table>
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<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>$U_{11}$</th>
<th>$U_{22}$</th>
<th>$U_{33}$</th>
<th>$U_{12}$</th>
<th>$U_{13}$</th>
<th>$U_{23}$</th>
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<td>Si(1)</td>
<td>0.3647(3)</td>
<td>0.2508(3)</td>
<td>0.3825(5)</td>
<td>139(12)</td>
<td>138(14)</td>
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<td>0.3680(3)</td>
<td>0.1021(5)</td>
<td>111(11)</td>
<td>132(14)</td>
<td>71(12)</td>
<td>64(10)</td>
<td>31(9)</td>
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<td>Si(3)</td>
<td>0.7596(3)</td>
<td>0.1251(4)</td>
<td>0.7688(5)</td>
<td>134(12)</td>
<td>174(14)</td>
<td>70(12)</td>
<td>97(11)</td>
<td>34(9)</td>
<td>32(10)</td>
<td>110(10)</td>
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<td>Ca</td>
<td>0.6211(4)</td>
<td>0.9328(4)</td>
<td>0.1730(6)</td>
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<td>178(14)</td>
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<td>95(12)</td>
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<td>0.9776(15)</td>
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<td>180(39)</td>
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<td>0.3189(16)</td>
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<td>40(35)</td>
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<td>-29(27)</td>
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<td>0.5040(15)</td>
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<td>128(38)</td>
<td>106(30)</td>
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<td>0.2760(16)</td>
<td>227(36)</td>
<td>121(38)</td>
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<td>72(30)</td>
<td>3(30)</td>
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<tr>
<td>O(9)</td>
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<td>0.2935(14)</td>
<td>0.2480(22)</td>
<td>510(61)</td>
<td>462(68)</td>
<td>352(60)</td>
<td>449(58)</td>
<td>-137(48)</td>
<td>-57(49)</td>
<td>422(53)</td>
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<td>OW</td>
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<td>0.6984(20)</td>
<td>0.2675(27)</td>
<td>415(63)</td>
<td>872(119)</td>
<td>451(82)</td>
<td>318(75)</td>
<td>103(57)</td>
<td>169(78)</td>
<td>577(74)</td>
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</table>

* $U_{ij}$ and $U$ values are listed $\times 10^4$.
The chains share corners with the Si₆O₁₈ rings to form unshared edges (range 2.85 to 3.65 Å, mean 3.31 Å). The chains share corners with the Si₆O₁₈ rings to form a three-dimensional framework.

| TABLE 3 | SELECTED INTERATOMIC DISTANCES (Å) AND ANGLES (°) FOR GERENITE-(Y) |
| O(1)–O(2) | 1.05 | 0.50 | 0.27 | 2.05 |
| O(1)–O(3) | 1.11 | 0.59 x 2 | 0.29 | 2.01 |
| O(1)–O(4) | 0.88 | 1.01 | 0.46 x 2 | 0.48 | 2.00 |
| O(8)–O(9) | 1.07 | 0.44 x 2 | 0.46 | 1.99 |
| O(7)–O(8) | 1.10 | 0.56 | 0.26 | 1.91 |
| O(7)–O(8) | 1.01 | 0.42 | 1.99 |
| O(8)–O(9) | 1.09 | 0.05 | 0.28 | 2.04 |
| OW–OW | 0.28 | 0.25 |

Note: 〈O–O〉 denotes the mean metal-ligand distance (Å). Equivalent positions: x = x + 1, y = y + 1, z = z + 1; a = x + 1, y = y + 1, z = z + 1; c = x + 1, y = y + 1, z = z + 1; h = x + 1, y = y + 1, z = z + 1.

The atom at the Ca position is coordinated by eight anions, forming a distorted hexagonal dipyramid (Fig. 3). Bond-valence analysis (Table 4) shows that one of the apical anions (OW) is a molecule of H₂O, which contributes 0.26 valence units to the atom at the Ca position. The Ca–O₅H₂O distances range from 2.346 to 2.994 (mean 2.578 Å); those to the apical O(1) and OW atoms are 2.370 and 2.374 Å, respectively. The O–Ca–O₅H₂O angles vary from 53.8 to 128.8° (mean 90.0°). The polyhedron’s volume is 26.95 Å³.

The Ca positions are located just beyond and between pairs of Si₆O₁₈ rings. The Caₓ₁₂ (ϕ: unspecified anion) dipyramid shares opposite equatorial O(3)(1)–O(6) (2.85 Å) and O(3)(2)–O(3)(3) (3.13 Å) edges with Y(2) and Y(1) octahedra, respectively, from different chains. Adjacent equatorial O(1)–O(8) (2.58 Å) and O(3)–O(8) (2.59 Å) edges are shared with Si(1) and Si(3) tetrahedra, respectively, from one Si₆O₁₈ ring. The opposite O(2)–O(8) (2.61 Å) and O(6)–O(8) (2.64 Å) edges are shared with Si(1) and Si(3) tetrahedra, respectively, from another Si₆O₁₈ ring located above or below (±Z) the first. The dipyramid shares one non-equatorial O(1)–O(3) (3.18 Å) edge with the Y(2) octahedron adjacent to the Y(1) octahedron mentioned previously, and three other non-equatorial edges with other Ca polyhedra. The apical O(1) atom is also shared with an Si(3) atom in a third Si₆O₁₈ ring (located in the ±x direction), in addition to the Y(2) octahedron, and another Ca atom. The apical OW atom is located above or below the center of the closest Si₆O₁₈ ring, at a distance of ±1.82 and 0.48 Å from the planes formed by the Si and non-bridging O positions, respectively. There are two OW positions associated with each Si₆O₁₈ ring. As noted previously, bond-valence analysis shows that the “atom” at the OW position is a molecule of H₂O. The most likely acceptor for hydrogen bonding is another molecule of H₂O at an adjacent OW position associated with a different Si₆O₁₈ ring; the OW–OW distance is 2.80 Å. Other possibilities include oxygen...
Fig. 1. The structure of gerenite-(Y) projected onto (001). The SiO$_4$ tetrahedra are ruled, the Y(1)O$_6$ octahedra are indicated by a regular dot pattern, and the Y(2)O$_6$ octahedra, by a random-dot pattern. The Ca atoms are shown as circles with crosses, and the H$_2$O molecules, as open circles.

Fig. 2. The structure of gerenite-(Y) projected onto (010). The shading is the same as in the previous figure.

Fig. 3. Coordination of the Ca position in gerenite-(Y).
atoms at O(4) (2.97 Å) and O(9) (3.07 Å) positions. The Ca–OW–O(4) and Ca–OW–O(9) angles are 125.6° and 132.0°, respectively. However, the O(4)–OW–O(9) angle is only 92.5°, and the bond-valence sums to the O(4) and O(9) positions (Table 4) indicate that they are not involved in hydrogen bonding. A final possibility is another O(4) oxygen atom at a distance of 3.12 Å. However, it is unlikely that this is an acceptor, given the distance, the Ca–OW–O(4) angle of 89.1°, and the bond-valence sum to the O(4) position. Thus, the most likely acceptor for hydrogen bonding is the molecule of H₂O at an adjacent OW position.

**DISCUSSION**

The ideal formula of gerenite-(Y) is (Ca₄Na)₂(Y,REE)₃Si₅O₁₈•2H₂O. The empirical formula of gerenite, based on the electron-microprobe data in Jambor et al. (1998), and calculated on the basis of six Si atoms (H₂O by stoichiometry), is (Ca₁·₂Na₀·₅₇Mn₀·₀₆)₂₁·₇₈(Y₂₂·₂₂Dy₀·₁₉Er₀·₁₇Yb₀·₀₅Gd₀·₀₅Ho₀·₀₅Sm₀·₀₂Tb₀·₀₂Tm₀·₀₂Lu₀·₀₂Ce₀·₀₁Nd₀·₀₁)₄₂·₉₉Si₆O₁₈H₄·₀₀. The formula based on the structure analysis is (Ca₁·₂₁Na₀·₅₇)₂₁·₇₈(Y₂·₂₄REE₀·₆₈)₄₂·₉₉Si₆O₁₈•2H₂O. It is interesting to note that selected results of electron-microprobe analyses of non-intergrowth gerenite-(Y) crystals show a Ca:Na ratio approximately 1:1 (Jambor et al. 1998); this may indicate fully occupied Ca and Y sites in these particular grains.

The results of the crystal-structure analysis show two H₂O molecules per formula unit, corresponding to approximately 4.1 wt.% H₂O. This is similar to the 3.9 wt.% obtained by Jambor et al. (1998) using the Penfield method, but much less than the 6.0 wt.%
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FIG. 5. The structure of leifite projected onto (001) (top) and (100) (bottom), as adapted from Coda et al. (1974). The SiO₄ tetrahedra are ruled, the BeO₄ tetrahedra are indicated by crosses, the Na atoms are shown as ruled circles, and the H₂O molecules, as open circles.

According to the classification scheme of Liebau (1985), gerenite-(Y) belongs to the group of silicates with unbranched single rings of the form [Si₆O₁₈]²⁻, which also includes baratovite, beryl, combeite, diopside, imandrite, kazakovite, petaragite, scawtite, tourmaline, zirconsialite, and synthetic Na₆Sn(Si₆O₁₈) (Liebau 1985).

Because most gerenite-(Y) occurs intergrown with kainosite-(Y) and quartz at the type locality, and because the intergrowths may be pseudomorphic after leifite (Miller 1996, Jambor et al. 1998), it is interesting to compare the structure of gerenite-(Y) with those of kainosite-(Y) and leifite. The structure of kainosite-(Y), Ca₂(Y,Ce)₂(SiO₃)₆(CO₃)₂·H₂O, was solved by Rumanova et al. (1967) and refined by Giuseppetti et al. (1989). They showed that the structure consists of [Si₆O₁₈]²⁻ rings and CO₃ groups oriented approximately parallel to (001), and occupying “holes” in a framework made up of (Y,REE) and Ca polyhedra that alternately form sheets parallel to (010) (Fig. 4). Unlike gerenite-(Y), the atoms at the (Y,REE) positions are coordinated by eight O atoms forming a distorted dodecahedron; the mean bond-length is 2.385 Å, and the polyhedron volume is 23.57 Å³. Like gerenite-(Y), the atoms at the Ca positions are coordinated by eight anions; however, the resulting polyhedron is a distorted dodecahedron rather than a dipyramid. The mean bond-distance is 2.385 Å, and the polyhedron volume is 23.57 Å³; these are somewhat smaller than the corresponding values for gerenite-(Y) (2.578 Å and 26.95 Å³, respectively). Similar to gerenite-(Y), one of the anions coordinating the Ca position is an H₂O molecule; the Ca-H₂O distance is 2.505 Å [compared to 2.374 Å in gerenite-(Y)].

obtained by static heating tests of a bulk sample, and the 6.89 wt.% obtained by difference from the average analytical total in the electron-microprobe analyses.

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The crystal structure of leifite, Na6Be2Al2Si6O30(\text{OH})2•1.5H2O, was determined by Coda et al. (1974), who showed that there are two Si, one (Si,Al), and one Be sites, all in tetrahedral coordination with oxygen (Fig. 5). The (Si,Al) tetrahedra (occupied by approximately 2/3 Si and 1/3 Al) form six-membered rings parallel to (001). However, the centers of the rings are much farther apart (14.352 Å) than in gerenite-(Y) (-9.5 or 12.6 Å, the latter measured diagonally across the unit cell), because in leifite they are linked by Si and Be tetrahedra, which gives rise to additional chains and rings. There are H2O molecules at the centers of the six-membered rings, and Na atoms occupy irregular seven-coordinated sites within the three-dimensional framework of Si and Be tetrahedra. Electron-microprobe analyses by Petersen et al. (1994) showed excess (Na,K) atoms that presumably could be accommodated in place of the H2O molecules. Wet-chemical and infrared spectroscopic analyses by Larsen & Åsheim (1995) showed excess K atoms and no H2O. The leifite structure was classified by Liebau (1985) as a tectosilicate, but with an interrupted (open-branched zweiter) framework.

It is interesting to note the similarities that exist among the structures of gerenite-(Y), kainosite-(Y) (the Ca9 polyhedron and the H2O position) and leifite (six-membered rings). This implies a paragenetic relationship between the three minerals, as suggested by their spatial relationship at the type locality.

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**References**


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