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β-$Y_2Si_2O_7$, a new thortveitite-type compound, determined at 100 and 280 K

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A new form of $Y_2Si_2O_7$ (diyttrium heptaoxodisilicate) has been synthesized which is isotypic with thortveitite, $Sc_2Si_2O_7$, and crystallizes in the centrosymmetric space group *C*2/*m*, both at 100 and 280 K. The Y^{3+} cation occupies a distorted octahedral site, with Y—O bond lengths in the range 2.239 (2)–2.309 (2) Å. The SiO_4 tetrahedron is remarkably regular, with Si—O bond lengths in the range 1.619 (2)–1.630 (2) Å. The bridging O atom of the Si_2O_7 pyrosilicate group shows a large anisotropic displacement perpendicular to the Si—O bond. Changes in lattice and structural parameters upon cooling are small with, however, a distinct decrease of the anisotropic displacement of the briding O atom. Structure solution and refinement in the non-centrosymmetric space group *C*2 are possible but do not yield a significantly different structure model. The Si—O—Si bond angle of the isolated Si_2O_7 groups is 179.2 (1)° at 280 K in *C*2 and 180° per symmetry in *C*2/*m*. The *C*2/*m* structure model is favoured.

Comment

Thortveitite, $Sc_2Si_2O_7$, is one of the few scandium minerals representing silicates with isolated Si_2O_7 groups (sorosilicates). A unique feature of the thortveitite structure is the unusual Si—O—Si angle, which is reported to be 180° (Kimata *et al.*, 1998; Bianchi *et al.*, 1988; Smolin *et al.*, 1973; Cruickshank *et al.*, 1962). There has been considerable discussion about the correctness of this structure model, as the value of 180° is rather unusual for sorosilicates, where the corresponding angles are usually much smaller (130–140°; Liebau, 1986). This discussion was also concerned with the question of whether the correct space group for thortveitite is *C*2/*m*, *C*2 or *Cm*, all of which are possible on the basis of the diffraction symmetry. It was concluded, however, that the correct space group is *C*2/*m*, as it provides the most consistent bond lengths and angles, in spite of an Si—O—Si angle of 180° (Bianchi *et al.*, 1988; Smolin *et al.*, 1973; Cruickshank *et al.*, 1962). The *C*2 structural model provided by Cruickshank *et al.* (1962) yields Si—O—Si angles of about 165°.

The present structure determination of $Y_2Si_2O_7$, (I), confirms the structural similarity of this particular polymorph to thortveitite. The structure of (I) consists of sheets of YO_6 octahedra perpendicular to the crystallographic *c* axis and separated by the Si_2O_7 pyrosilicate groups, which run parallel to the *a* axis. Fig. 1 shows an ellipsoid plot with the atomic nomenclature of (I) and Fig. 2 shows a polyhedral representation of the structure viewed along [001].

All the YO_6 octahedra in (I) share three edges with each other and form a distorted honeycomb arrangement. The Y—O bond lengths are in the range 2.239 (2)–2.309 (2) Å, with an average value of 2.256 Å. The octahedral site in (I) is significantly larger than that in $Sc_2Si_2O_7$ (mean Sc—O bond length of 2.123 Å; Smolin *et al.*, 1972), but comparable with that in $Yb_2Si_2O_7$ (mean Yb—O bond length of 2.240 Å; Christensen, 1994). These differences in the average octahedral bond lengths reflect the differences in ionic radii of Y^{3+} (0.89 Å), Yb^{3+} (0.86 Å) and Sc^{3+} (0.72 Å) in octahedral coordination (Shannon & Prewitt, 1969). The deviations of the individual bond lengths from their mean value are small in (I) [BLD (bond-length distortion) = 0.38%] but the quadratic variance of the octahedral angles (OAV; Robinson *et al.*, 1971) is very high (OAV = 219.2°), revealing that Y^{3+} occupies a very much distorted octahedral environment. Similar octahedral distortion parameters are also found for $Yb_2Si_2O_7$ (BLD = 0.44% and OAV = 215.2°) and $Sc_2Si_2O_7$ (BLD = 0.58% and OAV = 216.0°).

The isolated Si_2O_7 groups in (I) are packed in columns along the *a* axis. As mentioned above, the unusual feature of the thortveitite structure is the existence of collinear Si—O1—Si bonds, as the bridging O1 atom is located at a centre of symmetry at $(0,0,\frac{1}{2})$. Each terminal O atom (two O2 and one O3) of the SiO_4 tetrahedron is also part of two YO_6 octahedra. The triangular faces defined by the terminal O atoms in adjacent SiO_4 groups are oriented in opposite directions. These tetrahedra are markedly regular in (I). The Si—O bond

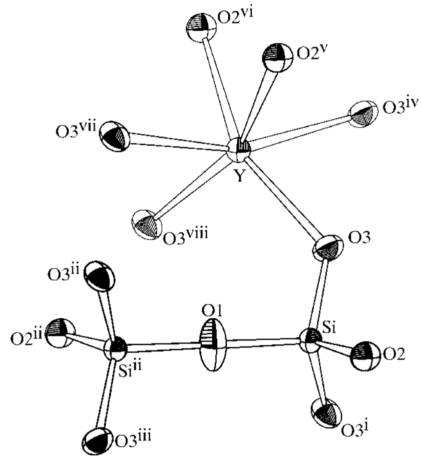

Figure 1
A view of the structure of (I) at 280 K, with 95% probability displacement ellipsoids [symmetry codes: (i) $x, -y, z$; (ii) $-x, y, 1-z$; (iii) $-x, -y, 1-z$; (iv) $\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z$; (v) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (vi) $x-\frac{1}{2}, \frac{1}{2}+y, z-1$; (vii) $x-\frac{1}{2}, \frac{1}{2}-y, z$; (viii) $-x, y, -z$].

lengths vary between 1.619 (2) and 1.630 (2) Å, with an average value of 1.627 Å, which is slightly larger than the average Si—O bond length in $Sc_2Si_2O_7$ (1.624 Å; Smolin *et al.*, 1973). The tetrahedral bond-length distortion in (I) is small (BLD = 0.24%) and about half the value calculated for $Sc_2Si_2O_7$ (BLD = 0.55%; Smolin *et al.*, 1973). Contrary to other thortveitite-type compounds, the Si—O1 bond in (I) (bridging the two pyrosilicate groups) is not the shortest; the shortest is the Si—O2 bond. The Si—O1 bond length is about 0.010–0.015 Å longer in (I) than, for instance, in synthetic $Sc_2Si_2O_7$ (Si—O1 = 1.606 Å; Smolin *et al.*, 1972) or in $In_2Si_2O_7$ (Si—O1 = 1.608 Å; Patzke *et al.*, 2000). It is the longer Si—O1 bond which reduces the BLD in (I) compared with the other compounds investigated to date. In addition to the BLD, the SiO_4 tetrahedra in (I) are also more regular in terms of the tetrahedral angle variance (TAV; Robinson *et al.*, 1971). The TAV is 4.63° in (I) compared with 8.3–14.1° in other natural and synthetic thortveitites. This difference is due to a smaller O2—Si—O3 angle in (I) and a larger (more ideal) O1—Si—O2 angle, which is 106.25 (10)° in (I) but ranges between 103.5 and 104.8° in natural (Bianchi *et al.*, 1988; Kimata *et al.*, 1998) and synthetic thortveitites (Smolin *et al.*, 1973).

A striking feature of (I) is the rather large anisotropic displacement parameter of the bridging O1 atom. There is a strong component of motion perpendicular to the Si—O1 bond, reflecting some displacement with respect to the linkage of the individual SiO_4 tetrahedra. For their natural thortveitite sample, *i.e.* $(Sc_{1.693}Y_{0.181}Yb_{0.095}Fe_{0.031})Si_2O_7$, Kimata *et al.* (1998) found by bond-length–bond-strength calculations that the bridging O1 atom possesses an oversaturation of 2.12 valence units. The authors argued that large atomic displacements may arise from either overbonding or underbonding. Overbonding supposedly directs repulsive energy to the nearest-neighbour atom, resulting in dynamic positional disorder. The correlation between overbonding of the bridging O1 atom and its large anisotropic thermal motion is also valid for the four natural thortveitites studied by Bianchi *et al.* (1988) and for the synthetic thortveitite of Smolin *et al.* (1973). This correlation, however, does not hold true for $Y_2Si_2O_7$, where atom O1 is saturated [bond-valence sum (Σs) = 1.98], atom O2 is slightly overbonded (Σs = 2.16) and atom O3 appears to be underbonded (Σs = 1.83). [Bond-valence calculations were performed using the parameters of Brese & O'Keeffe (1991) and Brown & Altermatt (1985).]

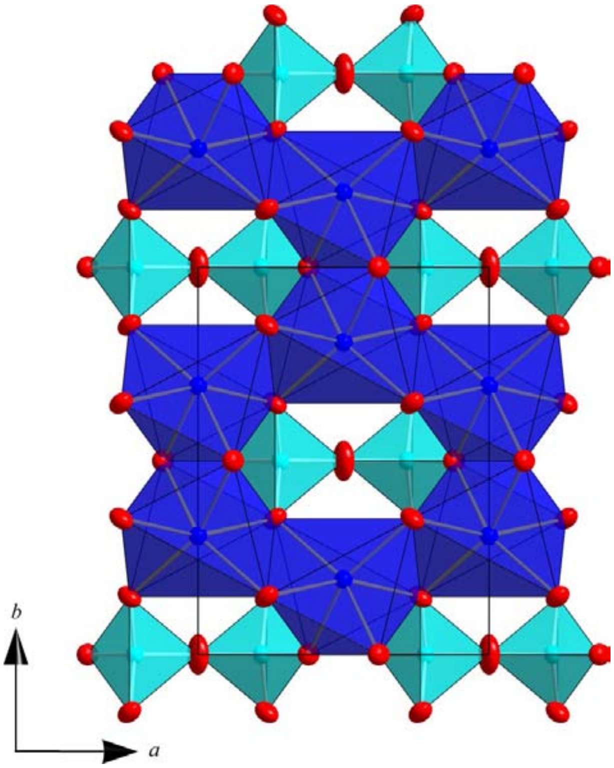

Figure 2
The structure of (I) at 280 K viewed down the [001] direction, showing the distorted honeycomb arrangement of the YO_6 octahedra.

The structure of (I) was also investigated at 100 K, revealing only very minor changes (*i.e.* one standard uncertainty or less) in lattice parameters and bond lengths. On the other hand, the anisotropic displacement parameters of all atoms decreased significantly (20–50%) between 280 and 100 K. The most pronounced reduction in anisotropy occurs for the bridging O1 atom of the Si_2O_7 group, for which U_{22} decreases from 0.0286 (19) Å^2 at 280 K to 0.0126 (15) Å^2 at 100 K, and the U_{22}/U_{11} ratio correspondingly drops by almost a factor of 2.

Since the first structure determination of $Sc_2Si_2O_7$ by Zachariasen (1930), several silicate compounds belonging to the thortveitite structure type have been synthesized and their complete structural data reported. These include $Yb_2Si_2O_7$ (Christensen, 1994), $Pr_2Si_2O_7$ (Felsche, 1971) and $In_2Si_2O_7$ (Reid *et al.*, 1977; Gaewdang *et al.*, 1994; Patzke *et al.*, 2000). For (I), the thortveitite structure type has not been described to date, although the compound has been described in the literature. Ito & Johnson (1968) noted that $Y_2Si_2O_7$ shows four polymorphic forms (α, β, γ and δ) with increasing temperature, following the sequence $\alpha \rightarrow \beta$ (1498 K), $\beta \rightarrow \gamma$ (1718 K) and $\gamma \rightarrow \delta$ (1808 K). The α, β, γ and δ polymorphs correspond to the *B*, *C*, *D* and *E* types defined by Christensen (1994). The γ phase is monoclinic, space group $P2_1/m$ (Batalieva & Pyatenko, 1971). The δ phase is orthorhombic, with *Pnam* (Diaz *et al.*, 1990) or $Pna2_1$ symmetry (Smolin & Shepelev, 1970; Christensen, 1994). Diaz *et al.* (1990) noted that the γ phase transforms to an 'α' phase with $C2/m$ symmetry below 1718 K. This 'α'-$Y_2Si_2O_7$ was described earlier by Batalieva *et al.* (1967), but no detailed structural data are available for this phase in the literature. It has to be noted here that, in both papers, the $C2/m$ phase is wrongly identified as the α phase. Instead, this polymorph corresponds to the β phase, as shown by the excellent match of its lattice parameters with those determined by Ito & Johnson (1968) for the β phase. Since the lattice parameters of (I) are very close to those given by Batalieva *et al.* (1967), with the same $C2/m$ space group, it is concluded that (I) corresponds to β-$Y_2Si_2O_7$. On the other hand, α-$Y_2Si_2O_7$ is triclinic and, although no structural data have been reported to date, it is probably isotypic with triclinic α-$Ho_2Si_2O_7$ (Felsche, 1972) and $Dy_2Si_2O_7$ (Fleet & Liu, 2000). In contrast with the thortveitite structure, the structure of

$Dy_2Si_2O_7$ contains linear triple tetrahedral $[Si_3O_{10}]$ groups and isolated $[SiO_4]$ tetrahedra, which are crosslinked by Dy^{3+} in one sixfold- and three eightfold-coordinated positions (Fleet & Liu, 2000). Therefore, the structural topologies of the α and β phases of $Y_2Si_2O_7$ seem to be quite distinct.

As mentioned before, β-$Y_2Si_2O_7$ ($C2/m$) transforms to γ-$Y_2Si_2O_7$ ($P2_1/m$) and the structural topologies of these polymorphs are rather different from each other. In γ-$Y_2Si_2O_7$, the layers of YO_6 octahedra are still present, but the honeycomb arrangement observed in (I) is broken up. Instead, chains of *cis*-connected and edge-sharing YO_6 octahedra are formed parallel to the *a* axis. These chains are linked by common corners in the *b* direction *via trans* O atoms to form layers parallel to the *ab* plane. The γ-$Y_2Si_2O_7$ structure contains two different Y sites (within and between the octahedral chains), which are distinct in terms of polyhedral distortion (for the Y1 site, BLD = 2.1% and OAV = 352.4°; for the Y2 site, BLD = 0.5% and OAV = 262.3°) and which are both significantly underbonded (Σs = 2.65 and 2.46 for Y1 and Y2, respectively). Another striking difference between the β and γ polymorphs of $Y_2Si_2O_7$ is the arrangement of the pyrosilicate groups. Whereas the Si—O—Si angle is 180° in the β phase, it is only 134° in the γ phase (Batalieva & Pyatenko, 1971). The latter contains two different tetrahedral sites, which are more distorted than in the β phase (for the Si1 site, BLD = 1.2% and TAV = 25.2°; for the Si2 site, BLD = 0.9% and TAV = 51.8°). Bond-valence calculations show that the bridging O atom of the pyrosilicate group in the γ phase is saturated (Σs = 2.02), with adequate bond-valence sums around atoms Si1 (Σs = 3.91) and Si2 (Σs = 4.11). [It has been noted that the Inorganic Crystal Structure Database (2003) entry for γ-$Y_2Si_2O_7$ (28004) contains a typing error for the *z* coordinate of atom O5, which should read 0.736 instead of 0.786.]

At about 1808 K, γ-$Y_2Si_2O_7$ transforms to orthorhombic ($Pnam$) δ-$Y_2Si_2O_7$, which is also structurally distinct from both the γ and β phases (Diaz *et al.*, 1990). The δ-$Y_2Si_2O_7$ structure contains only one symmetry-independent Y site which, in contrast with the other two polymorphs, is seven-coordinate and forms a net of edge- and corner-sharing YO_7 polyhedra. The δ phase also contains two symmetry-non-equivalent Si sites with similar tetrahedral angular distortions (for Si1, TAV = 68.4°; for Si2, TAV = 63.7°) but different bond-length distortions (BLD = 2.1 and 0.5%, respectively). Within the pyrosilicate groups, the Si—O—Si angle is 157.3° and the bridging O atom is saturated (Σs = 2.06). The bond-valence sum for the bridging O atom seems to increase slightly from the β to the γ and δ polymorphs, perhaps corresponding to the fact that this atom in δ-$Y_2Si_2O_7$ is not only bonded to the two Si atoms but also to the Y atom. Overall, among the three polymorphs of $Y_2Si_2O_7$, the thortveitite-type β phase contains the most regular YO_6 and SiO_4 polyhedra.

Experimental

Single crystals of $Y_2Si_2O_7$, (I), were obtained while attempting to synthesize the clinopyroxene compound $NaYSi_2O_6$ using high-temperature solution (flux) growth methods. Na_2CO_3, Y_2O_3 and SiO_2 were mixed in the proportions corresponding to the chemical composition of $NaYSi_2O_6$. The carefully ground powders were mixed with Na_2MoO_4 as a high-temperature flux (nutrient–flux ratio of 1:10) and placed in a covered platinum crucible. The crucible was slowly heated to 1473 K, kept at this temperature for 24 h and then slowly cooled (2 K h^{-1}) to 673 K. As synthesis experiments have shown, the clinopyroxene phase $NaYSi_2O_6$ is not stable under these experimental conditions and, after dissolving the molybdate flux in boiling water, the product consisted of colourless cuboid-shaped crystals of (I), large thin platelets of $Na_2Si_2O_5$ and colourless cuboid crystals of a yttrium orthosilicate oxyapatite which will be described elsewhere.

Compound (I) at 280 K

Crystal data

$Y_2Si_2O_7$
M_r = 345.98
Monoclinic, $C2/m$
a = 6.8691 (16) Å
b = 8.960 (2) Å
c = 4.7168 (11) Å
β = 101.730 (18)°
V = 284.26 (12) Å^3
Z = 2

D_x = 4.042 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2329 reflections
θ = 3.8–32.1°
μ = 20.72 mm^{-1}
T = 280 (1) K
Cuboid, pale yellow
0.17 × 0.15 × 0.14 mm

Data collection

Stoe IPDS-2 diffractometer
Rotation scans
Absorption correction: numerical *via* equivalents (*X-SHAPE* and *X-RED*; Stoe & Cie, 1996)
T_{min} = 0.054, T_{max} = 0.109
1672 measured reflections

520 independent reflections
497 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 32.2°
$h = -10 \rightarrow 9$
$k = -13 \rightarrow 11$
$l = -6 \rightarrow 6$

Refinement

Refinement on F^2
$R(F)$ = 0.019
$wR(F^2)$ = 0.045
S = 1.17
520 reflections
32 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0226P)^2 + 0.3813P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.068 (3)

Table 1
Selected geometric parameters (Å, °) for (I) at 280 K.

Y—O3^{i}	2.2386 (15)	Y—O3^{v}	2.3091 (17)
Y—O3	2.2386 (15)	Si—O2	1.619 (2)
Y—O2^{ii}	2.2479 (14)	Si—O1	1.6280 (9)
Y—O2^{iii}	2.2479 (14)	Si—O3^{vi}	1.6301 (17)
Y—O3^{iv}	2.3091 (17)	Si—O3	1.6301 (17)
O3^{i}—Y—O3	102.13 (9)	O3—Y—O3^{v}	117.13 (7)
O3^{i}—Y—O2^{ii}	155.39 (7)	O2^{ii}—Y—O3^{v}	79.81 (7)
O3—Y—O2^{ii}	93.54 (6)	O2^{iii}—Y—O3^{v}	84.82 (7)
O3^{i}—Y—O2^{iii}	93.54 (6)	O3^{iv}—Y—O3^{v}	160.08 (8)
O3—Y—O2^{iii}	155.39 (7)	O2—Si—O1	106.25 (10)
O2^{ii}—Y—O2^{iii}	78.84 (8)	O2—Si—O3^{vi}	111.70 (7)
O3^{i}—Y—O3^{iv}	117.13 (7)	O1—Si—O3^{vi}	108.40 (6)
O3—Y—O3^{iv}	76.19 (6)	O2—Si—O3	111.70 (7)
O2^{ii}—Y—O3^{iv}	84.82 (7)	O1—Si—O3	108.40 (6)
O2^{iii}—Y—O3^{iv}	79.81 (7)	O3^{vi}—Si—O3	110.21 (12)
O3^{i}—Y—O3^{v}	76.19 (6)	Si—O1—Si^{vii}	180.000 (13)

Symmetry codes: (i) $-x, y, -z$; (ii) $\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$; (iii) $x - \frac{1}{2}, \frac{1}{2} + y, z - 1$; (iv) $\frac{1}{2} - x, \frac{1}{2} - y, -z$; (v) $x - \frac{1}{2}, \frac{1}{2} - y, z$; (vi) $x, -y, z$; (vii) $-x, -y, 1 - z$.

Compound (I) at 100 K

Crystal data

$Y_2Si_2O_7$
$M_r = 345.98$
Monoclinic, $C2/m$
$a = 6.8667\ (16)$ Å
$b = 8.959\ (2)$ Å
$c = 4.7167\ (11)$ Å
$\beta = 101.724\ (18)^\circ$
$V = 284.11\ (12)$ Å^3
$Z = 2$

$D_x = 4.042$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2397 reflections
$\theta = 3.8$–32.1°
$\mu = 20.72$ mm^{-1}
$T = 100\ (1)$ K
Cuboid, pale yellow
0.17 × 0.15 × 0.14 mm

Data collection

Stoe IPDS-2 diffractometer
Rotation scans
Absorption correction: numerical *via* equivalents (*X-SHAPE* and X-*RED*; Stoe & Cie, 1996)
$T_{\min} = 0.057$, $T_{\max} = 0.111$
1660 measured reflections

518 independent reflections
499 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.042$
$\theta_{\max} = 32.2^\circ$
$h = -9 \rightarrow 10$
$k = -13 \rightarrow 10$
$l = -6 \rightarrow 6$

Refinement

Refinement on F^2
$R(F) = 0.021$
$wR(F^2) = 0.048$
$S = 1.12$
518 reflections
32 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0237P)^2 + 0.6763P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.75$ e Å^{-3}
$\Delta\rho_{\min} = -0.81$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.046 (3)

Table 2
Selected geometric parameters (Å, °) for (I) at 100 K.

Y—O3$^{\rm i}$	2.2369 (16)	Y—O3$^{\rm v}$	2.3070 (18)
Y—O3	2.2369 (16)	Si—O2	1.619 (2)
Y—O2$^{\rm ii}$	2.2461 (15)	Si—O1	1.6294 (9)
Y—O2$^{\rm iii}$	2.2461 (15)	Si—O3$^{\rm vi}$	1.6325 (18)
Y—O3$^{\rm iv}$	2.3070 (18)	Si—O3	1.6325 (18)
O3$^{\rm i}$—Y—O3	102.19 (9)	O3—Y—O3$^{\rm v}$	76.10 (7)
O3$^{\rm i}$—Y—O2$^{\rm ii}$	155.34 (8)	O2$^{\rm ii}$—Y—O3$^{\rm v}$	84.87 (8)
O3—Y—O2$^{\rm ii}$	93.54 (6)	O2$^{\rm iii}$—Y—O3$^{\rm v}$	79.86 (8)
O3$^{\rm i}$—Y—O2$^{\rm iii}$	93.54 (6)	O3$^{\rm iv}$—Y—O3$^{\rm v}$	160.21 (8)
O3—Y—O2$^{\rm iii}$	155.34 (8)	O2—Si—O1	106.23 (10)
O2$^{\rm ii}$—Y—O2$^{\rm iii}$	78.82 (9)	O2—Si—O3$^{\rm vi}$	111.79 (8)
O3$^{\rm i}$—Y—O3$^{\rm iv}$	76.10 (7)	O1—Si—O3$^{\rm vi}$	108.31 (7)
O3—Y—O3$^{\rm iv}$	117.13 (7)	O2—Si—O3	111.79 (8)
O2$^{\rm ii}$—Y—O3$^{\rm iv}$	79.86 (8)	O1—Si—O3	108.31 (6)
O2$^{\rm iii}$—Y—O3$^{\rm iv}$	84.87 (8)	O3$^{\rm vi}$—Si—O3	110.22 (13)
O3$^{\rm i}$—Y—O3$^{\rm v}$	117.13 (7)	Si$^{\rm vii}$—O1—Si	180

Symmetry codes: (i) $-x, y, -z$; (ii) $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$; (iii) $x-\frac{1}{2}, \frac{1}{2}+y, z-1$; (iv) $x-\frac{1}{2}, \frac{1}{2}-y, z$; (v) $\frac{1}{2}-x, \frac{1}{2}-y, -z$; (vi) $x, -y, z$; (vii) $-x, -y, 1-z$.

Structure solution using the 280 K data was initially performed in space group $C2$, as E statistics suggested a non-centrosymmetric space group ($E^2 - 1 = 0.745$). The non-centrosymmetric structural model found with the Patterson method could be refined down to $R1$(all) = 2.5% and $wR2$(all) = 5.3%. However, the displacement parameters for two of the four O atoms became non-positive definite. Validation tests of the final $C2$ structure model using the *ADDSYM* option of *PLATON* (Spek, 2003) clearly showed the presence of additional symmetry (mirror plane), suggesting that $C2/m$ was the correct space group. Thus, a new structure solution was tried, revealing the known thortveitite structure type and yielding better final residual values (with fewer refined parameters) and positive definite displacement parameters for all atoms, even for the data before absorption correction. The differences between the $C2/m$ and $C2$ structural models are very small. In $C2$, two different Y sites exist, Y1 and Y2. The Y1—O bond lengths vary between 2.231 (7) and 2.341 (7) Å (mean 2.274 Å) and the Y2—O bond lengths vary between 2.244 (7) and 2.285 (9) Å (mean 2.260 Å). The SiO_4 tetrahedron in the $C2$ structure is more distorted, with bond lengths ranging between 1.591 (9) and 1.659 (9) Å (mean 1.625 Å). In contrast with the $C2$ model reported by Cruickshank *et al.* (1962), our $C2$ model contains an Si—O—Si angle of 179.2 (1)°, and as in $C2/m$, the bridging O atom shows a large anisotropic displacement perpendicular to the Si—O bond.

For compound (I) at both 100 and 280 K, data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 1996); structure solution: *SHELXS*97 (Sheldrick, 1997); structure refinement: *SHELXL*97 (Sheldrick, 1997). For (I) at 280 K, molecular graphics: *DIAMOND* (Brandenburg & Berndt, 1999); preparation of publication material: *WinGX* (Farrugia, 1999).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: BC1023). Services for accessing these data are described at the back of the journal.

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