Crystal structure and compressibility of zircon at high pressure

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Abstract

Unit-cell and crystal-structure parameters of zircon (ZrSiO$_4$, tetragonal $I4_{1}$/amd, $Z$ = 4) have been determined at eight pressures from 1 bar to 48.1 kbar. Volume compressibility is $4.41 \pm 0.04 \times 10^{-4}$ kbar$^{-1}$ (bulk modulus $2.27 \pm 0.02$ Mbar), and linear compressibilities are $\beta_{\parallel} = 0.95 \times 10^{-4}$ and $\beta_{\perp} = 1.6 \times 10^{-4}$ kbar$^{-1}$. Zircon is less compressible than any other measured compound with tetrahedrally-coordinated silicon.

Projections of tetrahedral Si-O bond distances to high pressure suggest that $^{14}$Si to $^{16}$Si transformations occur when the tetrahedral distance compresses to approximately 1.59A, on the basis of known transformation pressures, Si-O bond compressibilities, and room-pressure structures of several silicates. For silicates with room-pressure Si-O distances ranging from 1.61 to 1.655A, predicted transformations to 6-coordinated silicon structures will occur between approximately 100 and 300 kbar at $23^\circ$C. These transformation pressures are relatively insensitive to temperature ($dP/dT \leq 0.01$ kbar/$^\circ$C), and $^{14}$Si to $^{16}$Si transitions are therefore predicted to occur primarily in the transition zone of high-density gradient of the earth's mantle. ZrSiO$_4$ is predicted to transform to a dense phase with octahedral silicon at approximately 170 kbar.

Introduction

Silicon-to-oxygen bonds are structural elements of many minerals throughout the earth's crust and mantle. The response of Si-O bonds to pressure, therefore, is an important parameter in characterizing the solid earth. Silicon is tetrahedrally coordinated in all known crustal silicates, but high-pressure transformations of silicates to forms with 6-coordinated silicon (stishovite, perovskite-type silicates) are well known. Liu (1978) has recently proposed that silicon might also enter 8-coordination in fluorite-like structures in the lower mantle, on the basis of high-pressure transformations of SnO$_2$ and TiO$_2$ to fluorite-related structures.

Bonds between oxygen and tetravalent cations have been characterized as rigid structural elements that change little, compared to weaker bonds, with changes in temperature or pressure. Zircon is an excellent structure to test this suggestion, for all metal cations are tetravalent. Furthermore, because of edge sharing between polyhedra, all changes in unit-cell volume must be accompanied by changes in metal-oxygen distances. The compressibility and thermal expansivity of zircon consequently should be among the lowest for oxygen-based compounds. The reported zircon volume thermal expansion is $1 \times 10^{-5}$ $^\circ$C$^{-1}$, which is significantly lower than that of most other silicates (typically $2-4 \times 10^{-5}$ $^\circ$C$^{-1}$; Clark, 1966). The reported bulk modulus of nonmetamict zircon is approximately $2.3$ Mbar (Ozkan and Jamieson, 1978), which is larger than values for olivines, garnets, silicate spinels, and other close-packed silicates (Clark, 1966).

The crystal structure of zircon was described and illustrated by Robinson et al. (1971), who cited earlier studies. Finger (1973) presented revised values of zircon structure parameters. The volume compressibility of zircon has been measured by several authors (Madelung and Fuchs, 1921; Ozkan and Jamieson, 1978; Singh and Kennedy, 1977). Of the previous workers, only Singh and Kennedy reported the axial compressibilities of this tetragonal mineral; however, their results have considerable scatter. The principal objective of our study was to determine the axial and volume compressibilities for zircon, to relate these compressions to changes in interatomic distances, and to compare these changes with those in other silicates at high pressure.
HAZEN AND FINGER: CRYSTAL STRUCTURE OF ZIRCON

Table 1. Zircon unit-cell parameters and refinement conditions

<table>
<thead>
<tr>
<th>Crystal No. 1</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$P$ (kbar)</td>
<td>$a$ (Å)</td>
<td>$c$ (Å)</td>
<td>Vol. (Å$^3$)</td>
<td>$c/a$</td>
<td>No. of independent observed reflections</td>
<td>Weighted $R^\ast$ (%)</td>
</tr>
<tr>
<td>1 atm - before $P$</td>
<td>6.6042(4)$\dagger$</td>
<td>5.9796(3)</td>
<td>260.80(3)</td>
<td>0.9054</td>
<td>5055</td>
<td>5.1</td>
</tr>
<tr>
<td>9.8(5)</td>
<td>6.5927(4)</td>
<td>5.9742(3)</td>
<td>259.66(2)</td>
<td>0.9062</td>
<td>74</td>
<td>2.7</td>
</tr>
<tr>
<td>28.9(5)</td>
<td>6.5737(4)</td>
<td>5.9638(5)</td>
<td>257.72(3)</td>
<td>0.9072</td>
<td>74</td>
<td>3.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Crystal No. 2</th>
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<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>10.0(1.0)</td>
<td>6.5942(4)</td>
<td>5.9740(1)</td>
<td>259.77(2)</td>
<td>0.9059</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17.4(5)</td>
<td>6.5849(3)</td>
<td>5.9693(1)</td>
<td>258.83(2)</td>
<td>0.9065</td>
<td>79</td>
<td>3.9</td>
</tr>
<tr>
<td>23.2(5)</td>
<td>6.5808(3)</td>
<td>5.9670(1)</td>
<td>258.37(2)</td>
<td>0.9067</td>
<td>79</td>
<td>3.2</td>
</tr>
<tr>
<td>37.1(5)</td>
<td>6.5650(3)</td>
<td>5.9583(5)</td>
<td>256.80(3)</td>
<td>0.9076</td>
<td>82</td>
<td>3.3</td>
</tr>
<tr>
<td>42.0(5)</td>
<td>6.5592(4)</td>
<td>5.9553(5)</td>
<td>256.22(3)</td>
<td>0.9079</td>
<td>81</td>
<td>2.5</td>
</tr>
<tr>
<td>48.1(5)</td>
<td>6.5587(5)</td>
<td>5.9551(4)</td>
<td>256.17(4)</td>
<td>0.9080</td>
<td>73</td>
<td>2.8</td>
</tr>
<tr>
<td>1 atm - after $P$</td>
<td>6.6027(9)</td>
<td>5.9776(5)</td>
<td>260.62(5)</td>
<td>0.9054</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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**Experimental**

**Specimen description**

Fragments of nonmetamict zircon from a colorless, gem-quality single crystal were kindly provided by G. L. Davis, Geophysical Laboratory. The specimen is from a kimberlite, Finsch Pipe, near Kimberley, South Africa, and has an age of 94 m.y., as determined by U/Pb dating (Davis, 1977). The zircon is nearly pure ZrSiO$_4$, with 1.2 weight percent HfO$_2$ and 26 ppm uranium.

**High-pressure techniques**

Two fragments, with the excellent parting characteristic of some kimberlite zircons, were used in high-pressure experiments. Crystal No. 1 was a rectangular (110) plate, 90 × 90 × 30 μm, and crystal No. 2 was a triangular (100) plate 100 μm on a side and 35 μm thick. Crystals were mounted in a miniature opposed-diamond pressure cell (Merrill and Bassett, 1974), using Inconel 750X (International Nickel Company, Inc.) gaskets, and 4:1 methanol:ethanol as the hydrostatic pressure medium. Ruby crystals of approximately 10 μm maximum dimension were included in the mount, and pressures were calibrated to ±0.5 kbar using the pressure shift of the $R_t$ ruby fluorescence line (Piermarini et al., 1975).

Details of procedures for crystal mounting, crystal centering on the four-circle diffractometer, unit-cell determination, and data collection are described elsewhere (Hazen, 1976; Finger and King, 1978; Hazen and Finger, 1977).

**Data collection and refinement**

Intensity measurements were made on an automated four-circle Picker diffractometer with Nb-filtered MoKα radiation, using the constant precision intensity technique described by Finger et al. (1973) and the fixed-φ mode of data collection at high pressure (Finger and King, 1978). All reflections in one octant of reciprocal space from 0.1 to 0.9 sin θ/λ were collected at room pressure, and all accessible reflections in one hemisphere of reciprocal space from 0.1 to 0.7 sin θ/λ were collected at high pressure. The number of independent observed reflections ($I > 2σ$), $R$ values, and unit-cell parameters are listed in Table 1. Zircon is tetragonal, but unit-cell parameters were refined without constraint to detect crystal strain. Unconstrained parameters were dimensionally tetragonal within two $esd$ at all pressures; at the highest pressure of 48 kbar, for example, $a_1 = 6.5531(3)$, $a_2 = 6.5531(17)$, $c = 5.9519(2)$, $α = 89.993(8)$, $β = 90.005(3)$, $γ = 89.984(12)$.

The observed intensities were corrected for absorp-
Table 2. Zircon refined fractional coordinates and anisotropic temperature factors

<table>
<thead>
<tr>
<th>Atom</th>
<th>Parameter</th>
<th>1 atm</th>
<th>9.8 kbar</th>
<th>17.4 kbar</th>
<th>23.2 kbar</th>
<th>28.9 kbar</th>
<th>37.1 kbar</th>
<th>42.0 kbar</th>
<th>48.1 kbar</th>
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</thead>
<tbody>
<tr>
<td>Zr*</td>
<td>$\mathbf{g}_{11}$</td>
<td>0.00171(9)+</td>
<td>0.0017(2)</td>
<td>0.0013(2)</td>
<td>0.0018(2)</td>
<td>0.0017(3)</td>
<td>0.0018(2)</td>
<td>0.0018(2)</td>
<td>0.0018(2)</td>
</tr>
<tr>
<td></td>
<td>$\mathbf{g}_{22}$</td>
<td>0.00161(13)</td>
<td>0.0023(5)</td>
<td>0.0023(5)</td>
<td>0.0020(3)</td>
<td>0.0012(6)</td>
<td>0.0020(2)</td>
<td>0.0027(2)</td>
<td>0.0021(3)</td>
</tr>
<tr>
<td>Si‡</td>
<td>$\mathbf{g}_{31}$</td>
<td>0.00171(9)</td>
<td>0.0031(5)</td>
<td>0.0020(6)</td>
<td>0.0021(5)</td>
<td>0.0025(5)</td>
<td>0.0028(5)</td>
<td>0.0026(4)</td>
<td>0.0017(6)</td>
</tr>
<tr>
<td></td>
<td>$\mathbf{g}_{33}$</td>
<td>0.00161(13)</td>
<td>0.0022(12)</td>
<td>0.0028(8)</td>
<td>0.0028(7)</td>
<td>0.0023(15)</td>
<td>0.0021(6)</td>
<td>0.0027(5)</td>
<td>0.004(7)</td>
</tr>
<tr>
<td>O‡‡</td>
<td>$\mathbf{g}$</td>
<td>0.066(4)</td>
<td>0.066(10)</td>
<td>0.066(10)</td>
<td>0.0657(9)</td>
<td>0.0653(7)</td>
<td>0.0656(8)</td>
<td>0.0656(7)</td>
<td>0.0659(9)</td>
</tr>
<tr>
<td></td>
<td>$\mathbf{z}$</td>
<td>0.193(4)</td>
<td>0.1962(8)</td>
<td>0.1963(9)</td>
<td>0.1952(8)</td>
<td>0.1954(9)</td>
<td>0.1962(7)</td>
<td>0.1960(6)</td>
<td>0.1958(8)</td>
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<tr>
<td></td>
<td>$\mathbf{g}_{11}$</td>
<td>0.0048(4)</td>
<td>0.0038(9)</td>
<td>0.0054(15)</td>
<td>0.0055(13)</td>
<td>0.0033(9)</td>
<td>0.0042(11)</td>
<td>0.0033(10)</td>
<td>0.0040(13)</td>
</tr>
<tr>
<td></td>
<td>$\mathbf{g}_{22}$</td>
<td>0.0022(4)</td>
<td>0.0043(9)</td>
<td>0.0040(13)</td>
<td>0.0038(12)</td>
<td>0.0029(10)</td>
<td>0.0040(10)</td>
<td>0.0040(8)</td>
<td>0.0022(13)</td>
</tr>
<tr>
<td></td>
<td>$\mathbf{g}_{31}$</td>
<td>0.0020(4)</td>
<td>0.0020(20)</td>
<td>0.0029(12)</td>
<td>0.0029(10)</td>
<td>0.0020(20)</td>
<td>0.0025(8)</td>
<td>0.0043(8)</td>
<td>0.0035(11)</td>
</tr>
<tr>
<td></td>
<td>$\mathbf{g}_{33}$</td>
<td>-0.0006(4)</td>
<td>0.000(8)</td>
<td>-0.0011(11)</td>
<td>0.0014(10)</td>
<td>-0.0001(8)</td>
<td>0.0012(8)</td>
<td>0.0003(7)</td>
<td>-0.0014(11)</td>
</tr>
</tbody>
</table>

*Zr is at (0,3/4,1/8). $g_{11} = g_{22}$ and $g_{12} = g_{13} = g_{23} = 0$.
‡Parenthesized figures represent e.s.d.'s of least units cited.
‡‡Si is at (0,1/4,3/8). $g_{11} = g_{22}$ and $g_{12} = g_{13} = g_{23} = 0$.
‡‡‡$\mathbf{g}$ = 0 and $g_{12} = g_{13} = 0$ for oxygen.

ion ($\mu = 44.3$ cm$^{-1}$), and refinement was accomplished using program REFIN (Finger and Prince, 1975)\(^1\). Neutral scattering factors of Cromer and Mann (1968) and coefficients for anomalous scattering of Cromer and Liberman (1970) were used for all atoms.

Zircon is tetragonal, space group $I4_1/amd$, with four ZrSiO$_4$ per unit cell. The structure has three atoms in the asymmetric unit, with Zr at (0,3/4,1/8), Si at (0,3/4,5/8), and O at (0,y,z). All refinements used a model with anisotropic temperature factors and an isotropic extinction correction. Anisotropic extinction corrections were refined for the room-pressure case but did not differ significantly from isotropic.

Results

Zircon compressibility

Regression analysis of unit-cell data in Table 1 yields equations that are linear in pressure (in kbar) from 0 to 50 kbar:

\[
\begin{align*}
a &= 6.6042(5) - 0.001062(2)P \\
c &= 5.9797(4) - 0.000572(2)P \\
V &= 260.79(4) - 0.1079(15)P
\end{align*}
\]

For each of the three curves, second-order coefficients are approximately half their estimated standard deviations, so there is no significant departure from linearity in this pressure range. The linear compressibility of $a$ ($1.6 \times 10^{-4}$ kbar$^{-1}$) is nearly twice that of $c$ ($0.95 \times 10^{-4}$ kbar$^{-1}$), causing an increase in $c/a$ with increasing pressure. The observed volume compressibility, $4.14(6) \times 10^{-8}$ kbar$^{-1}$, is similar to previously-reported values (Singh and Kennedy, 1977), and is the lowest value recorded for any mineral with silicon in tetrahedral coordination.

The calculated volume compressibility, $\beta$, and bulk modulus, $K_0 = 1/\beta$, vary slightly depending on the form of equation of state used. A simple polynomial fit yields $4.14(6) \times 10^{-4}$ kbar$^{-1}$ and 2.43(3) Mbar for $\beta$ and $K_0$ respectively, whereas second-order Murnaghan and Birch-Murnaghan equations of state with assumed $K_0'$ of 6.5 kbar (Özkan and Jamieson, 1978) yield $4.41(4) \times 10^{-4}$ kbar$^{-1}$ and 2.27(2) Mbar for $\beta$ and $K_0$. In either case, compressibility is significantly less than the 6.25-7.75 $\times 10^{-4}$ kbar$^{-1}$ values for other mantle silicates (Clark, 1966).

High-pressure crystal structure

Refined structural parameters for zircon at 1 bar, and 9.8, 17.4, 23.2, 28.9, 37.1, 42.0, and 48.1 (all ±0.5) kbar are presented in Table 2, and selected interatomic distances and angles are listed in Table 3. The two variable positional parameters (oxygen $y$ and $z$) do not vary within experimental error between 0 and 50 kbar. Changes in interatomic distances and angles, therefore, may be simply related to changes in the size of the unit cell. Weighted linear regression analysis of the metal–oxygen bond distances (in A) vs. pressure (in kbar) yields:

\[
\begin{align*}
d(\text{Si–O}) &= 1.622(1) - 0.00024(6)P \\
d(\text{Zr–O}) &= 2.268(1) - 0.00016(4)P \\
d(\text{Zr}^2\text{–O}) &= 2.1285(9) - 0.000306(4)P
\end{align*}
\]

Bond compressibilities are 1.48(37), 0.71(18), and 1.69(18) $\times 10^{-4}$ kbar$^{-1}$ for Si–O, Zr–O, and Zr$^2$–O,

---

\(^1\) Tabulated observed and calculated structure factors are available from the authors.
respectively. Polyhedral volume compressibilities are 0.44(11) and 0.36(6) Mbar\(^{-1}\) for the silicon tetrahedron and the zirconium dodecahedron, respectively.

The anisotropies in zircon unit-cell compression are a direct consequence of the anisotropic pressure response of the zirconium polyhedron. The Zr\(^{4+}\)-O bonds that are approximately parallel to \(a\) compress more than twice as much as the Zr-O bonds that are nearly parallel to \(c\). A major difference between Zr-O and Zr\(^{4+}\)-O bonds is that the oxygen atoms in Zr-O bonds form shared edges, whereas those in Zr\(^{4+}\)-O bonds are primarily corner-shared. The relative incompressibility of Zr-O bonds compared to Zr\(^{4+}\)-O bonds may thus be due to a combination of symmetry restraints and to R\(^{4+}\)-R\(^{4+}\) repulsion across the shared edge.

**Thermal ellipsoids**

Orientations and magnitudes of zircon thermal ellipsoids are presented in Table 4 for eight pressures. Thermal ellipsoids are sensitive to errors in absorption corrections, both from the zircon crystal and from the diamond cell. It is significant, therefore, that no variations are observed within experimental error for any thermal parameter between 0 and 50 kbar, in spite of the fact that the 1 bar data were collected in air, the 9.8 and 28.9 kbar data were collected on crystal No. 1 in one diamond cell, and the other high-pressure data were collected on crystal No. 2 in a different diamond cell.

**Discussion**

**Bulk moduli of R\(^{4+}\) polyhedra**

Compression data are now available for three types of R\(^{4+}\) polyhedra: \(^{11}\)Si\(^{4+}\), \(^{12}\)Si\(^{4+}\), and \(^{111}\)Zr\(^{4+}\). Bulk moduli of silicon tetrahedra in olivines, spinels, garnets, pyroxenes, phlogopite, gilletspe, and zircon are consistent with a value of 2.5(4) Mbar. The zirconium dodecahedron of this study has a bulk modulus of 2.8(3) Mbar. Stishovite, SiO\(_2\) with silicon in octahedral coordination, has a bulk modulus of 3.0 Mbar (Sato, 1977), which is also the bulk modulus of the silicon polyhedron (stishovite is an example of a constrained structure in which volume compression is directly related to polyhedral compression; Finger et al., 1977). Thus the simple relationship of increasing compressibility with increasing size found by Hazen and Prewitt (1977) does not appear to apply to polyhedra with tetravalent cations. For example, silicon tetrahedra, although the smallest of the three R\(^{4+}\) polyhedra examined, are the most compressible. The \(^{11}\)Si\(^{4+}\)-O bond, with a Pauling bond strength of 4/6, is more rigid than the \(^{12}\)Si\(^{4+}\)-O bond, with bond strength 4/4. This behavior may in part be due to oxygen-oxygen repulsion, for the mean O-O bond
distance in stishovite is only 2.4A, as opposed to
2.65A in silicon tetrahedra. Oxygen-oxygen repul-
sion does not explain, however, why the large zirco-
nium dodecahedron with bond strength 4/8 (O-O
mean distance = 2.8A) is less compressible than the
silicon tetrahedron. It is possible that R\(^{+}^{+}\)-O bonds
vary considerably in degree of covalency. If Si-O
bonds in tetrahedra are more covalent than octahed-
ral Si-O or dodecahedral Zr-O bonds, then the
potential minimum separation will be less well de-
finite and might permit greater compression of the
shorter \(^{IV}\)Si-O bond.

All metal-oxygen polyhedra with +1, +2, or +3
cations previously studied have polyhedral bulk mod-
uli significantly less than the three +4 cations de-
dscribed above. It is possible, therefore, to predict
qualitatively the pressure response of oxygen-based
compounds with both R\(^{+}^{+}\) and lower valence cations.
There is, however, no procedure now available for
predicting the relative values of the small but real
compressibilities of different R\(^{+}^{+}\) polyhedra.

**Tetrahedral-to-octahedral silicon transitions**

Recent high-pressure experiments have demon-
strated that silicon will enter 6-coordination in some
mantle phases (Ringwood, 1975). Coesite (SiO\(_{2}\); Si-O
= 1.61A), for example, transforms to stishovite at 80
kbar (Yagi and Akimoto, 1976). All silicates mea-
sured are observed to have similar mean tetrahedral
Si-O compressibilities of 1.3(2) \(\times\) 10\(^{-4}\) kbar\(^{-1}\), so the
predicted mean Si-O distance in coesite at the 80
kbar transition is approximately 1.59A. Enstatite
(MgSiO\(_{3}\); Si-O = 1.63A) transforms to an ilmenite-
type structure at about 250 kbar (Liu, 1976; Ito,
1977). The predicted Si-O distance for enstatite at
this transformation is again approximately 1.59A.
Olivine [(Mg,Fe)\(_{2}\)SiO\(_{4}\); Si-O = 1.65A] transforms to
a silicate spinel at pressures between 50 and 100 kbar.
At room pressure the silicate spinel Si-O bond dis-
tance is 1.655, and the Si-O compressibility is ap-
proximately 1.2 \(\times\) 10\(^{-4}\) kbar\(^{-1}\) (Finger, Hazen and
Yagi, in preparation). This phase transforms to a
perovskite structure at approximately 270 kbar (Liu,
1976), at which pressure the spinel Si-O distance is
projected to be 1.60A. Orthoclase and albite (Si-O
= 1.61A in ordered tetrahedra) transform to dense as-
semblages with octahedral silicon at approximately
100 kbar (Ringwood, 1975), and the projected Si-O
distance is once again 1.59A. It appears, therefore,
that for silicate transformations from 4-coordinated
to 6-coordinated silicon, the Si-O distance of the
phase with tetrahedral silicon does not compress be-
low 1.59A.

The longest recorded mean Si-O tetrahedral bond
distance is approximately 1.655A in silicate spinels
(Finger et al., 1977), whereas the shortest Si-O bonds
are approximately 1.61A in framework silicates. If
1.59A represents a minimum Si-O distance, then the
range of pressures at which transformations from 4-
to 6-coordinated silicon may occur is from about 100
kbar (for framework silicates) to about 300 kbar (for
orthosilicates). Temperature is observed to have rela-
tively little effect on the pressures of 4-to-6 trans-
formations (for coesite to stishovite the temperature
effect is 0.01 kbar/\(^{\circ}\)C; Yagi and Akimoto, 1976). The
range of 4-to-6 transformations, therefore, corre-
sponds to a depth in the earth of approximately 300
to 900 km, which is the transition region of rapidly increasing density with depth.

High-pressure transformations of zircon

The minimum Si-O distance may also be used to predict high-pressure transformation conditions for ZrSiO$_4$. Zircon is known to transform to the scheelite (CaWO$_4$) structure at approximately 120 kbar (Reid and Ringwood, 1969); these two structures are closely related, however, varying only slightly in the arrangement of silicon and zircon polyhedra, and it is plausible to assume that the 1 bar Si-O distances and compressibility are similar for the scheelite-like and zircon polymorphs. The Si-O bond should compress to 1.59Å at approximately 160 kbar. For higher pressures the scheelite-like phase will probably transform to a phase with 6-coordinated Si. Ringwood (1975) has suggested the KAlF$_4$ structure type as the post-scheelite form of ZrSiO$_4$. If a bulk modulus of 3 Mbar is assumed for octahedrally-coordinated silicon, the Si-O distance would compress from the 1 atm value of approximately 1.78Å (Baur and Khan, 1971) to 1.74Å at the proposed transition pressure of 160 kbar. If the Si-O polyhedron is regular, as observed for KAlF$_4$ (Brosset, 1938), the resulting cell would correspond to a volume reduction of 30 percent at the 160 kbar transition. Furthermore, the Zr-O polyhedron would be a cube with a Zr-O distance of 2.8Å. It appears, therefore, from predicted bond distances and unit-cell volume, that the KAlF$_4$ structure is quite reasonable for the post-scheelite phase of ZrSiO$_4$.

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References


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