First-principles prediction of a new high pressure polymorph of the BaSi$_2$ compound

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Received 18 February 2014
Revised 2 April 2014
Accepted 3 April 2014
Published 2 May 2014

In this paper, we present a study of the structural stability of BaSi$_2$ under high pressure based on first-principles calculations using the projector augmented wave method and generalized gradient approximation as implemented in the ABINIT code. The equations of state of three known polymorphs of BaSi$_2$ and four candidate structures are calculated along with their structural parameters and their enthalpies of formation. A new polymorph of BaSi$_2$, not yet reported experimentally, is found to be more stable than all the other structures at high pressure and 0 K. It corresponds to the MgZn$_2$-type (h) hexagonal structure with hP12 Pearson symbol (space group: P6$_3$/mmc). The stiffness coefficients $B_{ij}$ and elastic properties including bulk modulus $B_0$ with its first and second pressure derivative ($B'_0$, $B''_0$), Young’s modulus ($E$) and Poisson’s ratio ($\nu$) are computed using the stress–strain method.

Keywords: BaSi compound; crystal structure; phase transition; high pressure; first principles.
Fig. 1. Schematic representation of the Laves structures C15, C14 and C36.

1. Introduction

Silicides are of great interest from geophysical, technological and crystallochemical points of view.\textsuperscript{1} The ecologically friendly silicides have also received increasing attention in technological applications. Like many other compounds, they adopt different structures under different temperatures and/or pressures. This feature proved to be very interesting in tuning their physical properties. This is illustrated in the study of superconductivity in this class of compound.

BaSi$_2$ has three polymorphs: The first one is orthorhombic oP24 (BaSi$_2$-type structure, space group: $Pnma$) which is the most stable structure at ambient structure.\textsuperscript{2,3} The other two phases are obtained by increasing pressure and temperature: First, the cP12 cubic structure (SrSi$_2$-type, space group: P4$_3$2) obtained from the orthorhombic structure in the temperature range of 873 K to 1073 K and a pressure of 4 GPa\textsuperscript{3−5}; second, the trigonal hP3 structure (EuGe$_2$-type, space group: P-3m1)\textsuperscript{6} obtained from the orthorhombic structure at 1273 K and 4 GPa.\textsuperscript{7} These two structures are metastable at ambient conditions. The orthorhombic and cubic BaSi$_2$ are semiconductors while the trigonal BaSi$_2$ is a metal which shows superconductivity with an onset temperature of 6.8 K.\textsuperscript{8,9}

In the present work, we are particularly interested in the work of Imai \textit{et al.}\textsuperscript{10} in which they discovered the existence of a new phase named BaSi$_2$-IV, which appears at high pressures and especially at high temperatures (above 1473 K). However, the structure of this phase is still unknown. The appearance of an amorphous phase at high pressures should be noted according to the work of Mizuno \textit{et al.}\textsuperscript{11} These authors have carried out the high-pressure X-ray diffraction study of BaSi$_2$ to confirm the transformation of high-pressure phases up to 60 GPa at room temperature, and discovered pressure-induced amorphization beyond 10 GPa. Further research was carried out by Nishii \textit{et al.}\textsuperscript{12} where they performed precise X-ray scattering...
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experiments to study the structure of the amorphous phase with analysis of the bond distance by pair-distribution function up to 45 GPa.

In order to have a more precise idea about this phase, we used first-principles calculations to investigate the stability of several candidate structures which turned out interesting in a similar study on CaSi$_2$. Many AX$_2$ compounds crystallize in the Laves phases and specially in hexagonal C14 (MgZn$_2$ type, space group: $P6_3/mmc$), hexagonal C36 (MgNi$_2$ type, space group: $P6_3/mmc$) and cubic C15 (MgCu$_2$ type, space group: $Fd\bar{3}m$) structures according to the relation between the atomic radii of the constituent elements. The structures of these Laves phases are shown in Fig. 1. We are interested in the KHg$_2$ structure with oI12 Pearson symbol (space group: Imma) and the three main Laves phases: the MgCu$_2$ cubic structure with cF24 Pearson symbol, the MgNi$_2$-type hexagonal structure hP24 and the other hexagonal structure hP12 of MgZn$_2$. Our results showed that the last one is a new high-pressure stable phase.

2. First-Principles Methodology

Our calculations were performed using the ABINIT code which is based on the plane-wave pseudopotential approach in the framework of the density functional theory (DFT). We used the projector augmented-wave (PAW) method, and the generalized gradient approximations (GGA) to treat the exchange interactions and correlation effects. The GGA is implemented according to the Perdew–Burke–Ernzerhof (PBE) functional. The PAW atomic data sets for Barium and Silicon were generated with the Atom Paw code. The atomic orbitals treated as valence states were $5s^26s^25p^6$ and $3s^23p^2$ for Ba and Si, respectively. The electron states were expanded in plane waves with kinetic energy cut-offs of 400 eV, and the Brillouin zone sampling was performed in such a way that the number of $k$-points multiplied by the number of atoms in the unit cell was greater than $10^4$. A cold smearing of 0.1 eV was used. The above parameters enabled us to obtain a total energy convergence of 1 meV per atom (0.1 kJ/mol-atom).

Elastic constants are a mechanical property that can be directly evaluated by first-principles methods. It reflects the linear response of the lattice to small strain around equilibrium. By applying a series of strain pattern on a crystal in equilibrium, a first-principles method gives the resulted stress and total energy. By using the stress–strain method or fitting total energy–strain curves according to their elastic relationships, one gets the elastic constants of the crystal. In order to estimate the elastic properties and the stability of the considered structure, we used the strain–stress method in which the relaxed unit cell under hydrostatic stress tensor was linearly deformed, then the stress tensor was calculated self-consistently after relaxing forces. In the special case of hydrostatic pressure, the elastic stiffness coefficient tensor has the symmetry of the elastic stiffness constant tensor. We adopted the proposed criteria by Wang et al. based on the elastic stiffness coefficients $C_{ij}$. 

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Table 1. Strains used to calculate the elastic stiffness constants $\gamma = \pm 0.003$.

<table>
<thead>
<tr>
<th>Strain components (unlisted $e_i = 0$)</th>
<th>Determined combinations of $C_{ij}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_1 = e_2 = \gamma$</td>
<td>$C_{11} + C_{12}, C_{13}$</td>
</tr>
<tr>
<td>$e_1 = -e_2 = \frac{\gamma}{2}, e_6 = \sqrt{3} \gamma$</td>
<td>$C_{11} - C_{12}$</td>
</tr>
<tr>
<td>$e_3 = \gamma$</td>
<td>$C_{33}, C_{13}$</td>
</tr>
<tr>
<td>$e_5 = \gamma$</td>
<td>$C_{44}$</td>
</tr>
</tbody>
</table>

In our study, we are interested in the hexagonal structure so that the Bravais lattice vectors of the strained unit cell $\{a'_i\}$ are related to those of the unstrained $\{a_i\}$ by the following form:

$$\begin{pmatrix} a'_1 \\ a'_2 \\ a'_3 \end{pmatrix} = \begin{pmatrix} \sqrt{3}a \\ -\frac{1}{2}a \\ 0 \end{pmatrix} \begin{pmatrix} 1 + e_1 & \frac{1}{2}e_6 & \frac{1}{2}e_5 \\ \frac{1}{2}e_6 & 1 + e_2 & \frac{1}{2}e_4 \\ \frac{1}{2}e_5 & \frac{1}{2}e_4 & 1 + e_3 \end{pmatrix},$$

(1)

where $a$ and $c$ are the hexagonal cell parameters, and $e_1, e_2, \ldots, e_6$ are the six independent components of the symmetric strain tensor. We applied different sets of small strains as described in Table 1 with the corresponding set of determined $C_{ij}$.\(^{13}\)

The stress–strain $\sigma_i$ relations at a pressure $p$ are then given as follows:

$$\sigma_i = -p\delta_{ij}\xi_i + C_{ij}e_j,$$

(2)

$$\xi_i = \begin{cases} 1 & \text{if } i = 1.2.3 \\ 0 & \text{if } i = 4.5.6 \end{cases}$$

(3)

where $\delta_{ij}$ is the Kronecker delta and the $C_{ij}$ are the elastic stiffness coefficients.

For each strain tensor given in Table 1, the parameter $\gamma$ takes the two values $\pm 0.003$. The stress tensor with the set of components $\sigma_i(\gamma)$ is obtained with the positive value, while the set $\sigma_i(-\gamma)$ is obtained with the negative value. By subtracting the second set from the first, we obtain the $C_{ij}$ coefficients as follows:

$$C_{ij} = \frac{\sigma_i(\gamma) - \sigma_i(-\gamma)}{2\gamma\delta_{ij}}.$$  

(4)

3. Results and Discussion

We started the present investigation by computing the equilibrium lattice constants and bulk modulus of pure elements Ba and Si then BaSi$_2$. In order to check the reliability of our generated atomic data sets we compared them with experimental
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Table 2. Calculated crystallographic parameters compared with experimental values.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Prototype</th>
<th>Pearson symbol</th>
<th>Space group</th>
<th>Abinit GGA (This work)</th>
<th>Pwsf$^a$</th>
<th>Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ba</td>
<td>fcc</td>
<td>cF4</td>
<td>Im3m (229)</td>
<td>$a = 5.032$</td>
<td>5.061</td>
<td>5.023$^b$</td>
</tr>
<tr>
<td>BaSi$_2$</td>
<td>BaSi$_2$</td>
<td>oP24</td>
<td>Pnma (62)</td>
<td>$a = 9.055$</td>
<td>8.950</td>
<td>8.934$^c$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>$b = 6.774$</td>
<td>6.701</td>
<td>6.730$^d$</td>
</tr>
<tr>
<td>Si</td>
<td>diam</td>
<td>cF8</td>
<td>Fd$ar{3}$m (227)</td>
<td>$c = 11.610$</td>
<td>11.470</td>
<td>11.54$^e$</td>
</tr>
</tbody>
</table>

Typically, the EOS, as shown in Fig. 2, were obtained by calculating twenty first-principles data points for a given structure in a

$^a$Ref. 29, $^b$Ref. 30, $^c$Ref. 31, $^d$Ref. 32, $^e$Ref. 33.
Fig. 3. The volume as a function of the pressure of the BaSi$_2$ compound with the suspected phases.

![Graph showing the volume as a function of pressure](image)

Table 3. Calculated atomic volume ($V_0$, Å$^3$/atom), bulk modulus ($B_0$, GPa) and its pressure derivative ($B'$) for Ba and Si.

<table>
<thead>
<tr>
<th></th>
<th>Ba</th>
<th>Si</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CASTEP code</td>
<td>ABINIT code</td>
</tr>
<tr>
<td>$V_0$</td>
<td>53.863</td>
<td>63.710</td>
</tr>
<tr>
<td>$B_0$</td>
<td>10</td>
<td>8.9</td>
</tr>
<tr>
<td>$B'$</td>
<td>2.4</td>
<td>3.187</td>
</tr>
</tbody>
</table>

*Ref. 32

range of ± 10% of the equilibrium volume and sometimes more points were added in compression. For each point, both the external and internal degrees of freedom of the structure are fully relaxed at constant volume. The obtained set of points was then fitted to a Birch–Murnaghan 4th-order EOS. Then, in order to determine the structure of the BaSi$_2$ at high pressures, we performed the same calculations for the three main candidate Laves phases cF24, hP24 and hP12 together with the KHg$_2$-type structures oI12. The equations of state of these polymorphs are shown in Figs. 2 and 3. The calculated equilibrium volume $V$ and the bulk modulus $B_0$ with its first and second pressure derivatives are given in Tables 3 and 4. The results of Kitano et al.$^{32}$ are also given for comparison.

Our results are acceptable when compared with those of Kitano et al.$^{32}$ if we take into account the usual trends of LDA and GGA. LDA used by Ref. 32 overestimates
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Table 4. Calculated atomic volume ($V_0$, $\text{Å}^3$/atom), bulk modulus ($B_0$, GPa), with its first and second pressure derivatives ($B'$, GPa), ($B''$, GPa$^{-1}$) for BaSi\textsubscript{2} polymorphs.

<table>
<thead>
<tr>
<th>Structure</th>
<th>CASTEP code\textsuperscript{a}</th>
<th>ABINIT code (this work)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>oP24</td>
<td>oP24    cP12  hP3  hP12  hP24  cF24</td>
</tr>
<tr>
<td>$B_0$</td>
<td>53</td>
<td>49.1    52.4  49.1  41.3  41.4  49.5</td>
</tr>
<tr>
<td>$B'' \times 10^{-3}$</td>
<td>—</td>
<td>$-0.158$ $-0.313$ $-0.159$ $-0.201$ $-0.154$ $-0.513$</td>
</tr>
</tbody>
</table>

\textsuperscript{a}Ref. 32

the bonding, resulting in larger cohesive energies and shorter lattice parameters. GGA used in our work overcorrects the LDA’s underestimation of the bonding, resulting in smaller cohesive energies and larger lattice parameters which are closer to experimental data.

At zero pressure, among the considered polymorphs, BaSi\textsubscript{2} in the orthorhombic oP24 structure type is correctly predicted to be the ground-state structure, as shown in Fig. 2. Then, we have the cubic cP12 structure with an energy difference of 0.616 eV per atom, and finally, the trigonal hP3 structure with an energy difference of about 0.158 eV per atom.

The oI12 structure was previously thought to be a new high-pressure polymorph, according to a similar work on CaSi\textsubscript{2} by Bouderba\textsuperscript{13} but it turned out that the Laves structure was more appropriate to be inspected for a new high-pressure polymorph. As shown in Fig. 2, the equations of state of the Laves structures and their equilibrium volumes, at zero pressure, are very close to each other and, as expected, their close-packed structures give the smallest equilibrium volumes as compared to the other structures. Also, as expected, the first Laves phase hP12 turned out to be the most stable. Then, with an energy difference by about 15 meV per atom, we find the hP24 phase and finally, the cF24 phase with an energy difference of 5 meV per atom. Thus, from the relative disposition of the three last curves (Laves structures) it is very important to note that the effect of the temperature is essential. Although the hP12 phase is the ground state among the Laves structures, the other structures are very close energetically and vibrational properties are expected to affect decisively the relative stabilities at finite temperature. It would be also interesting to investigate superconducting properties of these hypothetical Laves phases.

The structural phase stability is determined by calculating the Gibbs free energy for all structures, the stable phase being the one possessing the lowest energy:

$$G = E_{\text{tot}} + PV - TS,$$

where $E$, $S$, $P$ and $V$ are internal energy, vibrational entropy, pressure and volume, respectively. Since in theoretical calculations, we are only considering the zero-
Fig. 4. Enthalpy as a function of the pressure of BaSi$_2$ with the candidate phases.

temperature limit, Gibbs free energy is equal to enthalpy:

$$H = E_{\text{tot}} + PV,$$  \hspace{1cm} (6)

where $P = -\frac{\partial E}{\partial V}$.

At a given pressure, the stable structure is the one whose enthalpy has the lowest value and the transition pressure is calculated where the two phases have equal enthalpies.\(^{35,36}\) The relative stability of different structures of BaSi$_2$ can be deduced from the pressure dependence of enthalpy as shown in Fig. 4: the oP24 $\rightarrow$ cP12 $\rightarrow$ hP3 phase transitions occur at 0.74 GPa and 3.73 GPa, respectively. We must emphasize that our calculations were performed at 0 K. Regarding the experimental values, as reported by Imai \textit{et al.},\(^7\)\(^-\)\(^9\) both transitions occur at 4 GPa, but at different temperatures (873 K and 1273 K, respectively). Unfortunately, as far as we know, there are no theoretical results available related to the structural phase transition in the literature. We had no choice but to compare our results to the experimental data of Nishii \textit{et al.}\(^{12}\) In that work, they reveal that the amorphous phase appeared beyond 13 GPa and the Bragg peaks from the crystal phase almost disappeared at 15 GPa, which agrees well with our results. As shown in Fig. 2, the common tangent construction reveals that a predicted phase transition oP24 $\rightarrow$ hP12 occurs at 6.88 GPa, a value below the threshold of the occurrence of amorphism, which is consistent with the results of Nishii \textit{et al.} Since our
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Table 5. Calculated elastic stiffness coefficients of the hP12 structure at transition pressure (6.88 GPa). Results are given in GPa.

<table>
<thead>
<tr>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{13}$</th>
<th>$C_{33}$</th>
<th>$C_{44}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>164.594</td>
<td>48.417</td>
<td>78.859</td>
<td>229.359</td>
<td>89.981</td>
</tr>
</tbody>
</table>

calculations were performed at 0 K, the effect of temperature was not taken into account in our study.

In order to check the mechanical stability of the predicted high-pressure polymorph of the BaSi$_2$ (hP12, MgZn$_2$-type) we calculated its elastic stiffness constants (Table 5). These values satisfy all the stability conditions for hexagonal structures given by Ref. 37:

\[
\begin{align*}
C_{11} &> 0 \\
C_{44} &> 0 \\
C_{11} - C_{12} &> 0 \\
(C_{11} + C_{12})C_{33} - 2C_{13}^2 &> 0
\end{align*}
\]

Furthermore, according to the elastic constants obtained, we can compute the bulk modulus $B_0$ for the hexagonal phases, at the transition pressure, as follows:

\[
B_0 = \frac{C_{33}(C_{11} + C_{12}) - 2C_{13}^2}{C_{11} + C_{12} + 2C_{33} - 4C_{13}}.
\]

From the single crystal elastic constants, the polycrystalline elastic modulus is also estimated by the Voigt–Reuss–Hill (VRH) approximation.\textsuperscript{38,39} The Voigt and Reuss approximations represent the maximum and minimum limits of the polycrystalline elastic modulus, respectively. For hexagonal systems, the Voigt bounds of $B$ and $G$ are

\[
B_V = \frac{2}{9}\left(C_{11} + 2C_{12} + \frac{C_{33}}{2} + 2C_{13}\right),
\]

\[
G_V = \frac{1}{30}\left(7C_{11} - 5C_{12} + 2C_{33} - 4C_{13} + 12C_{44}\right).
\]

While the Reuss bounds are

\[
B_R = \frac{(C_{11} + C_{12})C_{33} - 2C_{13}^2}{C_{11} + C_{12} + 2C_{33} - 4C_{13}},
\]

\[
G_R = \frac{5}{2}\left(\frac{|(C_{11} + C_{12})C_{33} - 2C_{13}^2|C_{44}}{3B_VC_{44}C_{66} + |(C_{11} + C_{12})C_{33} - 2C_{13}^2|C_{44} + C_{66}}\right),
\]

\[
B = \frac{1}{2}(B_V + B_R),
\]

\[
G = \frac{1}{2}(G_V + G_R),
\]
Table 6. Elastic moduli (in GPa) and Poisson’s ratio for BaSi$_2$ (hp12) using Voigt, Reuss and Hill’s approximations.

<table>
<thead>
<tr>
<th>$B_0$</th>
<th>$B_V$</th>
<th>$G_V$</th>
<th>$B_R$</th>
<th>$G_R$</th>
<th>$B$</th>
<th>$G$</th>
<th>$E$</th>
<th>$G/B$</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>102.22</td>
<td>107.87</td>
<td>71.10</td>
<td>102.22</td>
<td>67.18</td>
<td>105.04</td>
<td>69.14</td>
<td>170.10</td>
<td>0.65</td>
<td>0.23</td>
</tr>
</tbody>
</table>

where $C_{66} = \frac{1}{2}(C_{11} - C_{12})$. The subscripts $V$ and $R$ designate the Voigt and the Reuss bounds, respectively.

In addition, Young’s modulus ($E$) and Poisson’s ratio ($\nu$) can be obtained from the bulk modulus and the shear modulus as follows:

$$E = \frac{9BG}{3B + G}, \quad (15)$$

$$\nu = \frac{3B - 2G}{2(3B + G)}, \quad (16)$$

The calculated results are shown in Table 6. In the literature, we do not have any theoretical results or experimental data related to these polycrystalline elastic moduli ($B_V, G_V, B_R, G_R, B, G, E, \nu$) in order to make a comparison with our results.

4. Conclusion

In this work, we have extensively explored the high-pressure crystal structure of polymeric BaSi$_2$ by first-principles calculations, using the projector augmented-wave (PAW) method within the density functional theory (DFT). The stiffness coefficients $B_{ij}$ and elastic properties including the bulk modulus $B_0$, its first and second pressure derivatives ($B', B''$), Young’s modulus ($E$) and Poisson’s ratio ($\nu$) for BaSi$_2$ polymorphs were calculated using the stress–strain method. We have shown that BaSi$_2$ has three high pressure phases. The phase transitions oP24 $\rightarrow$ cP12 $\rightarrow$ hP3 are in good agreement with the experimental data. We have also found that the new polymorph of BaSi$_2$ appear at 6.88 GPa and has hP12 structure (considering the transition oP24 $\rightarrow$ hP12) which agrees with the experimental work of Nishii et al.$^{11}$ This structure is most stable among the four structures studied. The current results may be taken as a starting point for further experimental or computational investigations.

Acknowledgments

The financial support of the Algerian General Direction for Scientific Research and Technological Development (PNR No. 8/u05/4532) is gratefully acknowledged. The Inorganic Material Database (http://crystdb.nims.go.jp/crystdb) was used to obtain some crystallographic data of some structures.
Appendix A

Table A.1. Calculated cell parameters of the orthorhombic and the hypothetical Laves phases of the BaSi$_2$ compound.

<table>
<thead>
<tr>
<th>Prototype</th>
<th>Symbol</th>
<th>Space Group</th>
<th>Lattice Parameters ($\text{A}$)</th>
<th>Atom Coordinates</th>
<th>Atom Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>MgCu$_2$</td>
<td>CF24</td>
<td>Fd$\bar{3}$m</td>
<td>$a = 11.652$</td>
<td>Ba 0 0 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$c = 9.165$</td>
<td>Si 5/8 5/8 5/8</td>
<td></td>
</tr>
<tr>
<td>MgZn$_2$</td>
<td>hP12</td>
<td>P6$_3$/mmc</td>
<td>$a = 6.153$</td>
<td>Ba$_1$ 1/3 2/3 0.04949</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$c = 6.153$</td>
<td>Si$_1$ 0 0 0</td>
<td></td>
</tr>
<tr>
<td>MgNi$_2$</td>
<td>hP24</td>
<td>P6$_3$/mmc</td>
<td>$a = 6.0.31$</td>
<td>Ba$_2$ 1/3 1/3 0.8446</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$c = 18.462$</td>
<td>Si$_1$ 1/3 2/3 0.2111</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Si$_2$ 1/2 0 0</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Si$_3$ 0.2003 0.4006 1/4</td>
<td></td>
</tr>
<tr>
<td>BaSi$_2$</td>
<td>oP24</td>
<td>Pnma</td>
<td>$a = 9.055$</td>
<td>Ba$_1$ 0.01406 1/4 0.69210</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$b = 6.774$</td>
<td>Ba$_2$ 0.84281 1/4 0.09389</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$c = 11.610$</td>
<td>Si$_1$ 0.41538 1/4 0.09064</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Si$_2$ 0.19815 1/4 0.96604</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Si$_3$ 0.19437 0.07216 0.14560</td>
<td></td>
</tr>
</tbody>
</table>

References

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34. http://elk.sourceforge.net/