

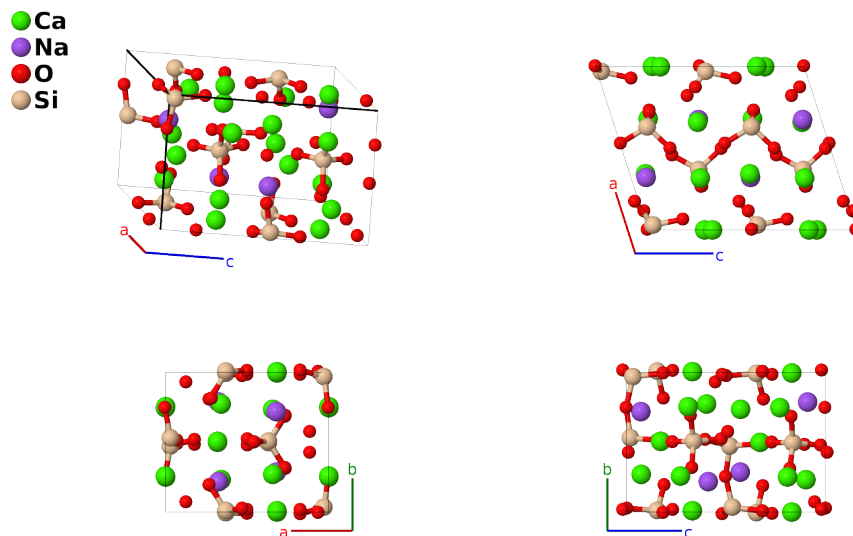
Na₂Ca₆Si₄O₁₅ Structure: A6B2C15D4_mP54_7_6a_2a_15a_4a-001

This structure originally had the label A6B2C15D4_mP54_7_6a_2a_15a_4a. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://afLOW.org/p/5V2T>

https://afLOW.org/p/A6B2C15D4_mP54_7_6a_2a_15a_4a-001

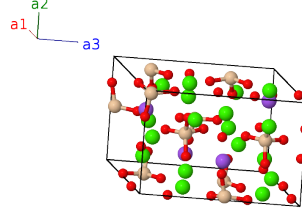


Prototype	Ca ₆ Na ₂ O ₁₅ Si ₄
AFLOW prototype label	A6B2C15D4_mP54_7_6a_2a_15a_4a-001
ICSD	256226
Pearson symbol	mP54
Space group number	7
Space group symbol	<i>Pc</i>
AFLOW prototype command	<pre>afLOW --proto=A6B2C15D4_mP54_7_6a_2a_15a_4a-001 --params=a, b/a, c/a, β, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁, x₁₂, y₁₂, z₁₂, x₁₃, y₁₃, z₁₃, x₁₄, y₁₄, z₁₄, x₁₅, y₁₅, z₁₅, x₁₆, y₁₆, z₁₆, x₁₇, y₁₇, z₁₇, x₁₈, y₁₈, z₁₈, x₁₉, y₁₉, z₁₉, x₂₀, y₂₀, z₂₀, x₂₁, y₂₁, z₂₁, x₂₂, y₂₂, z₂₂, x₂₃, y₂₃, z₂₃, x₂₄, y₂₄, z₂₄, x₂₅, y₂₅, z₂₅, x₂₆, y₂₆, z₂₆, x₂₇, y₂₇, z₂₇</pre>

- Although this structure was formed at 1300°C, the data was taken after cooling to room temperature, 295K.
- The true composition of the Ca-I site is Ca_{0.84}Na_{0.16}, and the Na-I site has composition Na_{0.84}Ca_{0.16}.
- The Si-III and Si-IV atoms share the O-X atom between them, accounting for the “missing” oxygen atom.

Simple Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	Ca I
\mathbf{B}_2	$x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Ca I
\mathbf{B}_3	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	Ca II
\mathbf{B}_4	$x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Ca II
\mathbf{B}_5	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	Ca III
\mathbf{B}_6	$x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Ca III
\mathbf{B}_7	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	Ca IV
\mathbf{B}_8	$x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Ca IV
\mathbf{B}_9	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	Ca V
\mathbf{B}_{10}	$x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Ca V
\mathbf{B}_{11}	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	Ca VI
\mathbf{B}_{12}	$x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Ca VI
\mathbf{B}_{13}	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	Na I
\mathbf{B}_{14}	$x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Na I
\mathbf{B}_{15}	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	Na II
\mathbf{B}_{16}	$x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_8 + c(z_8 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	Na II
\mathbf{B}_{17}	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	O I
\mathbf{B}_{18}	$x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_9 + c(z_9 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O I
\mathbf{B}_{19}	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(2a)	O II
\mathbf{B}_{20}	$x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_{10} + c(z_{10} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(2a)	O II
\mathbf{B}_{21}	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	=	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(2a)	O III

$$\mathbf{B}_{52} = x_{26} \mathbf{a}_1 - y_{26} \mathbf{a}_2 + \left(z_{26} + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} (ax_{26} + c(z_{26} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} + \\ c(z_{26} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} \quad (2a) \quad \text{Si III}$$

$$\mathbf{B}_{53} = x_{27} \mathbf{a}_1 + y_{27} \mathbf{a}_2 + z_{27} \mathbf{a}_3 = (ax_{27} + cz_{27} \cos \beta) \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} + cz_{27} \sin \beta \hat{\mathbf{z}} \quad (2a) \quad \text{Si IV}$$

$$\mathbf{B}_{54} = x_{27} \mathbf{a}_1 - y_{27} \mathbf{a}_2 + \left(z_{27} + \frac{1}{2}\right) \mathbf{a}_3 = \begin{pmatrix} (ax_{27} + c(z_{27} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_{27} \hat{\mathbf{y}} + \\ c(z_{27} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{pmatrix} \quad (2a) \quad \text{Si IV}$$

References

- [1] V. Kahlenberg and M. Maier, *On the existence of a high-temperature polymorph of $\text{Na}_2\text{Ca}_6\text{Si}_4\text{O}_{15}$ —implications for the phase equilibria in the system $\text{Na}_2\text{O}-\text{CaO}-\text{SiO}_2$* , *Miner. Petrol.* **110**, 903–915 (2016), doi:10.1007/s00710-016-0447-1.