

Sanidine (KAlSi₃O₈, *S*6₇) Structure: AB8C4_mC52_12_i_gi3j_2j-001

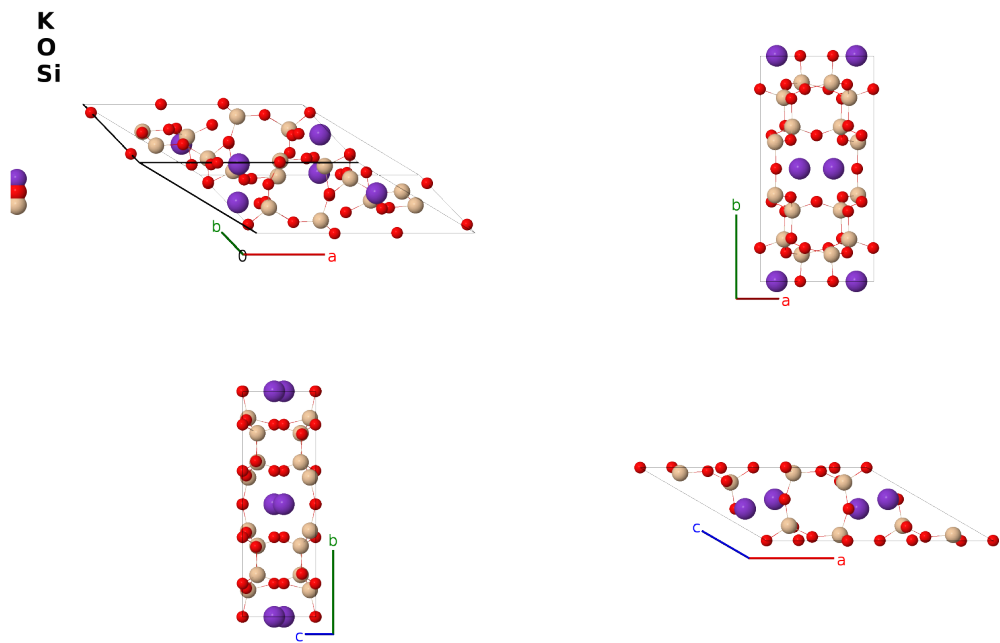
This structure previously used the label(s) **AB8C4_mC52_12_i_gi3j_2j**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/JF0M>

https://aflow.org/prototype-encyclopedia/AB8C4_mC52_12_i_gi3j_2j-001



Prototype	AlKO ₈ Si ₃
AFLOW prototype label	AB8C4_mC52_12_i_gi3j_2j-001
<i>Strukturbericht</i> designation	<i>S</i> 6 ₇
Mineral name	sanidine
ICSD	202476
CCDC	1707053
Pearson symbol	mC52
Space group number	12
Space group symbol	<i>C</i> 2/ <i>m</i>
AFLOW prototype command	<code>aflow --proto=AB8C4_mC52_12_i_gi3j_2j-001</code> <code>--params=a,b/a,c/a,β,y₁,x₂,z₂,x₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇,y₇,z₇,x₈,y₈,z₈</code>

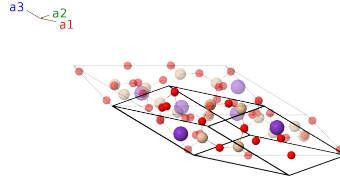
Other compounds with this structure

NaAlSi₃O₈, (BaKNa)AlSi₃O₈ (orthoclase)

- Beginning with the *S*67 defining paper of (Taylor, 1933) all researchers agree that the sites Si-I and Si-II are actually a random mixture of silicon and aluminum with overall stoichiometry AlSi₃. Most results found in (Downs, 2003) assume that this composition holds independently for both sites but (Scambos, 1987) states that the Si-I site is Al_{1.064}Si_{2.936} while the Si-II site is Al_{0.936}Si_{3.064}.
- (Scambos, 1987) list the coordinate $y_8 = 0.18813$ for the Si-II site in Table 2. This position does not result in the expected SiO₄ tetrahedra, and the interatomic distances and angles found do not agree with their Table 5. (Downs, 2003) correct this to $y_8 = 0.11813$, and this value results in good tetrahedra and reproduces the distances and angles reported by (Scambos, 1987). We use this later value on this page.

Base-centered Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$=$	$by_1 \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	$=$	$-by_1 \hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	K I
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4i)	K I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	O II
$\mathbf{B}_7$	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(8j)	O III
$\mathbf{B}_8$	$= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(8j)	O III
$\mathbf{B}_9$	$= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(8j)	O III
$\mathbf{B}_{10}$	$= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(8j)	O III
$\mathbf{B}_{11}$	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
$\mathbf{B}_{12}$	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
$\mathbf{B}_{13}$	$= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(8j)	O IV
$\mathbf{B}_{14}$	$= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8j)	O IV

$$\begin{aligned}
\mathbf{B}_{15} &= \frac{(x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3}{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}} & (8j) & \text{O V} \\
\mathbf{B}_{16} &= \frac{-(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3}{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}} & (8j) & \text{O V} \\
\mathbf{B}_{17} &= \frac{-(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3}{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}} & (8j) & \text{O V} \\
\mathbf{B}_{18} &= \frac{(x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3}{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}} & (8j) & \text{O V} \\
\mathbf{B}_{19} &= \frac{(x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3}{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}} & (8j) & \text{Si I} \\
\mathbf{B}_{20} &= \frac{-(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3}{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}} & (8j) & \text{Si I} \\
\mathbf{B}_{21} &= \frac{-(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3}{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}} & (8j) & \text{Si I} \\
\mathbf{B}_{22} &= \frac{(x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3}{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}} & (8j) & \text{Si I} \\
\mathbf{B}_{23} &= \frac{(x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3}{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}} & (8j) & \text{Si II} \\
\mathbf{B}_{24} &= \frac{-(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3}{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}} & (8j) & \text{Si II} \\
\mathbf{B}_{25} &= \frac{-(x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3}{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}} & (8j) & \text{Si II} \\
\mathbf{B}_{26} &= \frac{(x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3}{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}} & (8j) & \text{Si II}
\end{aligned}$$

References

- [1] T. A. Scambos, J. R. Smyth, and T. C. McCormick, *Crystal-structure refinement of high sanidine from the upper mantle*, Am. Mineral. **72**, 973–978 (1987).
- [2] W. H. Taylor, *The Structure of Sanidine and Other Felspars*, Z. Kristallogr. **85**, 425–442 (1933), doi:10.1524/zkri.1933.85.1.425.
- [3] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

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