α-Carnegieite ($NaAlSiO_4$, $S6_5$) Structure: ABC4D_cP28_198_a_a_ab_a-001

This structure originally had the label `ABC4D_cP28_198_a_a_ab_a`. Calls to that address will be redirected here.

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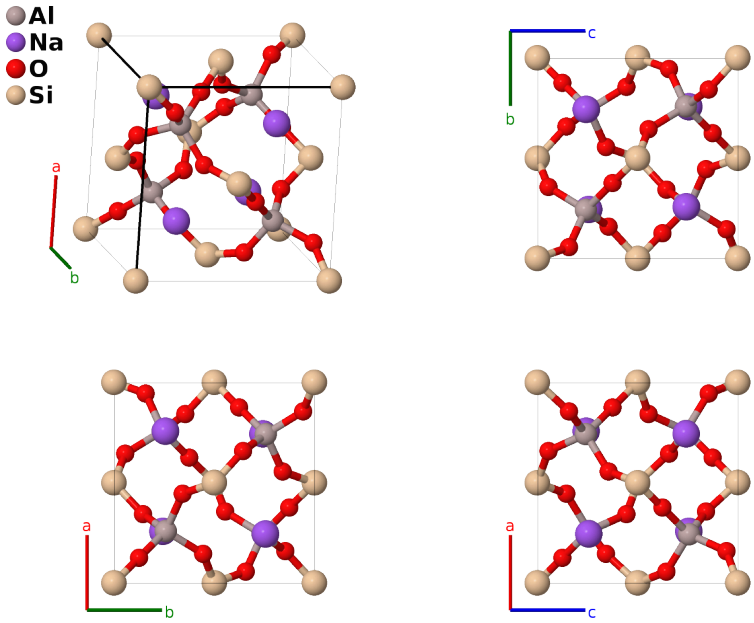
https://aflow.org/p/M6W2

https://aflow.org/p/ABC4D_cP28_198_a_a_ab_a-001

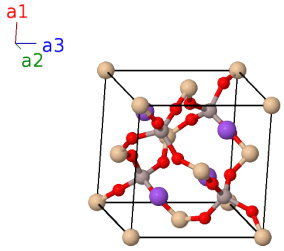


Prototype	$AlNaO_4Si$
AFLOW prototype label	ABC4D_cP28_198_a_a_ab_a-001
***Strukturbericht* designation**	$S6_5$
Mineral name	α-carnegieite
ICSD	34884
Pearson symbol	cP28
Space group number	198
Space group symbol	$P2_13$
AFLOW prototype command	`aflow --proto=ABC4D_cP28_198_a_a_ab_a-001 --params=`$a, x_1, x_2, x_3, x_4, x_5, y_5, z_5$

- This high-temperature form of carnegieite is stable above 970K.
- To our knowledge, the atomic positions of the low temperature β-carnegieite structure have not been determined.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{10}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_{14}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{18}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + a\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{19}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + a\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(z_5 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{20}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{21}}$	=	$z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ay_5\,\hat{\mathbf{z}}$	(12b)	O II

$\mathbf{B_{22}}$	=	$\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2-y_5\,\mathbf{a}_3$	=	$a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-ay_5\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{23}}$	=	$-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_1-x_5\,\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{24}}$	=	$-z_5\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{25}}$	=	$y_5\,\mathbf{a}_1+z_5\,\mathbf{a}_2+x_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}+az_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{26}}$	=	$-y_5\,\mathbf{a}_1+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}+a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{27}}$	=	$\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_2-x_5\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(12b)	O II
$\mathbf{B_{28}}$	=	$-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1-z_5\,\mathbf{a}_2+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-az_5\,\hat{\mathbf{y}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12b)	O II

References

[1] T. F. W. Barth and E. Posnjak, *Silicate structures of the cristobalite type: I. The crystal structure of α-carnegieite ($NaAlSiO_4$)*, Z. Kristallogr. **81**, 135–141 (1932), doi:10.1524/zkri.1932.81.1.135.