Sodalite [$Na_4(AlSiO_4)_3Cl$, $S6_2$] Structure: A3BC4D12E3_cP46_218_c_a_e_i_d-001

This structure previously used the label(s) `A3BC4D12E3_cP46_218_d_a_e_i_c`. Calls to these addresses will be redirected here.

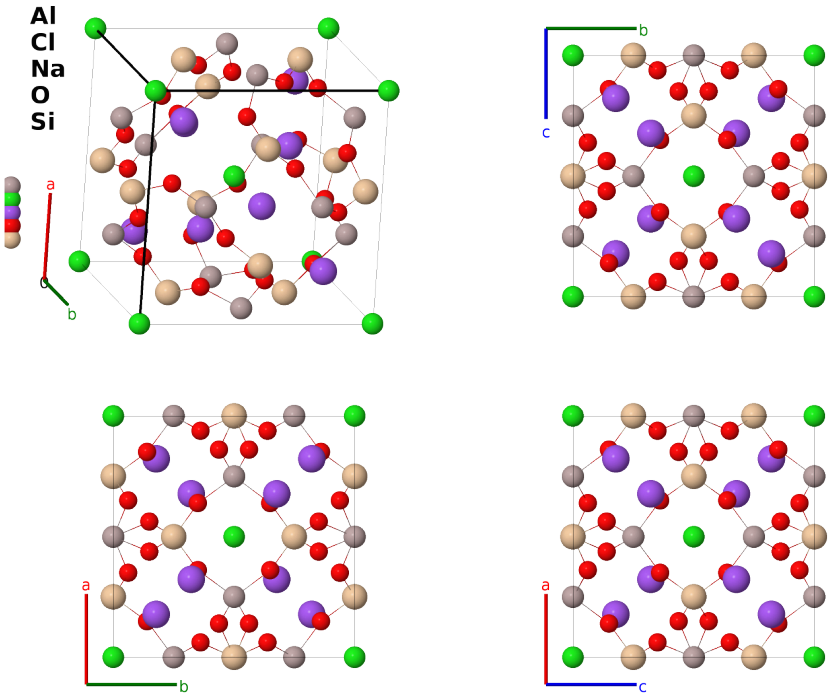
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/NYVB

https://aflow.org/prototype-encyclopedia/A3BC4D12E3_cP46_218_c_a_e_i_d-001



Prototype	$Al_3ClNa_4O_{12}Si_3$
AFLOW prototype label	A3BC4D12E3_cP46_218_c_a_e_i_d-001
***Strukturbericht* designation**	$S6_2$
Mineral name	sodalite
ICSD	29443
CCDC	1604408
Pearson symbol	cP46
Space group number	218
Space group symbol	$P\bar{4}3n$
AFLOW prototype command	`aflow --proto=A3BC4D12E3_cP46_218_c_a_e_i_d-001 --params=`a, x_4, x_5, y_5, z_5

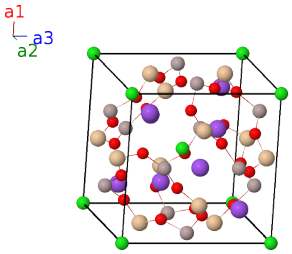
Other compounds with this structure

$(Na_xK_{1-x})_4(AlSiO_4)_3Cl$, $Li_4(AlSiO_4)_3Cl$, $(Li_xK_{1-x})_4(AlSiO_4)_3Cl$, $Na_4(AlSiO_4)_3Br$, $Na_4(AlSiO_4)_3I$

- Sodalites of the form $A_4(AlSiO_4)_3B$ with (A,B) = (Li,F), (Li,Br), (Li,I), (Na,F), (K,F), (K,Br) and (Rb,F) have been predicted to form, but not seen experimentally.

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
$\mathbf{B_1}$	=	0	=	0	(2a)	Cl I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(2a)	Cl I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(6c)	Al I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(6c)	Al I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(6c)	Al I
$\mathbf{B_9}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6d)	Si I
$\mathbf{B_{10}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6d)	Si I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(6d)	Si I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$	(6d)	Si I
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(6d)	Si I
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(6d)	Si I
$\mathbf{B_{15}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(8e)	Na I
$\mathbf{B_{16}}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(8e)	Na I
$\mathbf{B_{17}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(8e)	Na I
$\mathbf{B_{18}}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(8e)	Na I
$\mathbf{B_{19}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Na I
$\mathbf{B_{20}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Na I
$\mathbf{B_{21}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4-\frac{1}{2}\right)\,\mathbf{a}_2 - \left(x_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Na I

$\mathbf{B_{22}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	Na I
$\mathbf{B_{23}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}+az_5\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{24}}$	=	$-x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}+az_5\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{25}}$	=	$-x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}-az_5\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{26}}$	=	$x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2-z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}-az_5\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{27}}$	=	$z_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+y_5\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+ay_5\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{28}}$	=	$z_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2-y_5\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-ay_5\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{29}}$	=	$-z_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+y_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+ay_5\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{30}}$	=	$-z_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2-y_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-ay_5\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{31}}$	=	$y_5\,\mathbf{a}_1+z_5\,\mathbf{a}_2+x_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}+az_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{32}}$	=	$-y_5\,\mathbf{a}_1+z_5\,\mathbf{a}_2-x_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}+az_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{33}}$	=	$y_5\,\mathbf{a}_1-z_5\,\mathbf{a}_2-x_5\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}-az_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{34}}$	=	$-y_5\,\mathbf{a}_1-z_5\,\mathbf{a}_2+x_5\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}-az_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{35}}$	=	$\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{36}}$	=	$-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{37}}$	=	$\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{38}}$	=	$-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{39}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{40}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{41}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_2+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{42}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_2-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{43}}$	=	$\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{44}}$	=	$\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{45}}$	=	$-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O I
$\mathbf{B_{46}}$	=	$-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24i)	O I

References

[1] I. Hassan and H. D. Grundy, *The Crystal Structures of Sodalite-Group Minerals*, Acta Crystallogr. Sect. B **40**, 6–13 (1984), doi:10.1107/S0108768184001683.

First cited in

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.