

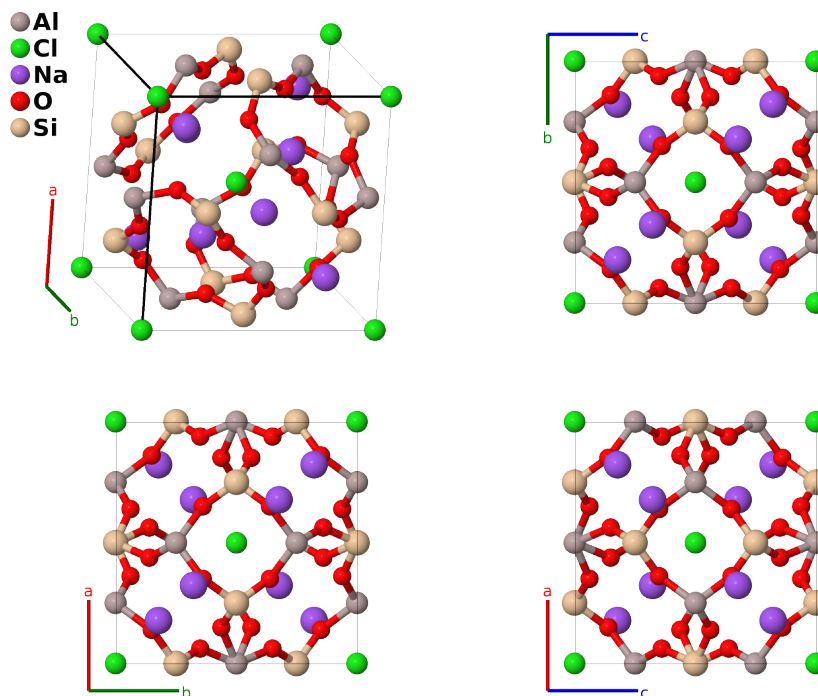
# Sodalite $[\text{Na}_4(\text{AlSiO}_4)_3\text{Cl}, S6_2]$ Structure: A3BC4D12E3\_cP46\_218\_c\_a\_e\_i\_d-001

This structure originally had the label A3BC4D12E3\_cP46\_218\_d\_a\_e\_i\_c. 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/NYVB>

[https://aflow.org/p/A3BC4D12E3\\_cP46\\_218\\_c\\_a\\_e\\_i\\_d-001](https://aflow.org/p/A3BC4D12E3_cP46_218_c_a_e_i_d-001)



Prototype	$\text{Al}_3\text{ClNa}_4\text{O}_{12}\text{Si}_3$
AFLOW prototype label	A3BC4D12E3_cP46_218_c_a_e_i_d-001
<i>Strukturbericht</i> designation	$S6_2$
Mineral name	sodalite
ICSD	29443
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

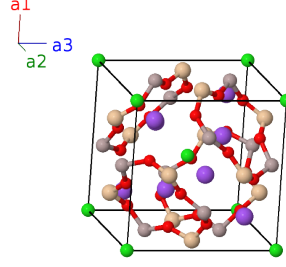
$(\text{Na}_x\text{K}_{1-x})_4(\text{AlSiO}_4)_3\text{Cl}$ ,  $\text{Li}_4(\text{AlSiO}_4)_3\text{Cl}$ ,  $(\text{Li}_x\text{K}_{1-x})_4(\text{AlSiO}_4)_3\text{Cl}$ ,  $\text{Na}_4(\text{AlSiO}_4)_3\text{Br}$ ,  $\text{Na}_4(\text{AlSiO}_4)_3\text{I}$

- 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.

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### Simple Cubic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}} \end{aligned}$$




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### 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
$\mathbf{B}_{19}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Na I
$\mathbf{B}_{20}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + (x_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Na I
$\mathbf{B}_{21}$	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 - (x_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Na I
$\mathbf{B}_{22}$	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(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

$$\begin{aligned}
\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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{O I}
\end{aligned}$$

## 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.