

NaAlCl₄ Structure:

AB4C_oP24_19_a_4a_a-001

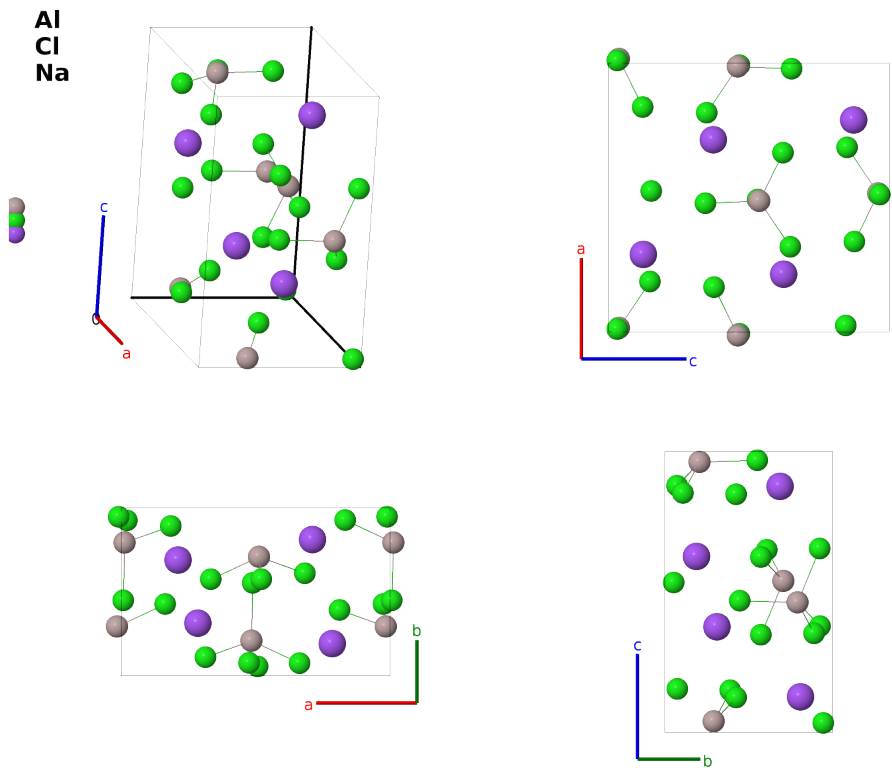
This structure previously used the label(s) **AB4C_oP24_19_a_4a_a**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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/43KD>

https://aflow.org/prototype-encyclopedia/AB4C_oP24_19_a_4a_a-001



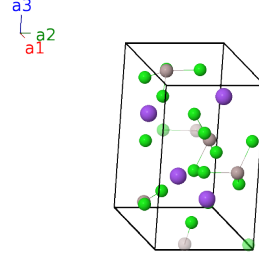
Prototype	AlCl ₄ Na
AFLOW prototype label	AB4C_oP24_19_a_4a_a-001
ICSD	8117
CCDC	1593905
Pearson symbol	oP24
Space group number	19
Space group symbol	$P2_12_12_1$
AFLOW prototype command	<pre>aflow --proto=AB4C_oP24_19_a_4a_a-001 --params=a,b/a,c/a,x₁,y₁,z₁,x₂,y₂,z₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆</pre>

Simple Orthorhombic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = b \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} + b \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(4a)	Cl I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4a)	Cl II
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cl II
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + b \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cl II
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(4a)	Cl II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4a)	Cl III
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - y_4 \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cl III
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} + b \left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cl III
$\mathbf{B}_{16}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$	(4a)	Cl III
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4a)	Cl IV
$\mathbf{B}_{18}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} + c \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cl IV
$\mathbf{B}_{19}$	$= -x_5 \mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} + b \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cl IV
$\mathbf{B}_{20}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_5 \hat{\mathbf{z}}$	(4a)	Cl IV

$$\begin{aligned}
\mathbf{B}_{21} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (4a) & \text{Na I} \\
\mathbf{B}_{22} &= -\left(x_6 - \frac{1}{2}\right) \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{Na I} \\
\mathbf{B}_{23} &= -x_6 \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right) \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{Na I} \\
\mathbf{B}_{24} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= a\left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (4a) & \text{Na I}
\end{aligned}$$

References

- [1] G. Mairesse, P. Barbier, and J.-P. Wignacourt, *Comparison of the crystal structures of alkaline ($M = \text{Li, Na, K, Rb, Cs}$) and pseudo-alkaline ($M = \text{NO, NH}_4$) tetrachloroaluminates, MAlCl_4* , Acta Crystallogr. Sect. B **35**, 1573–1580 (1979), doi:10.1107/S0567740879007160.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

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.