

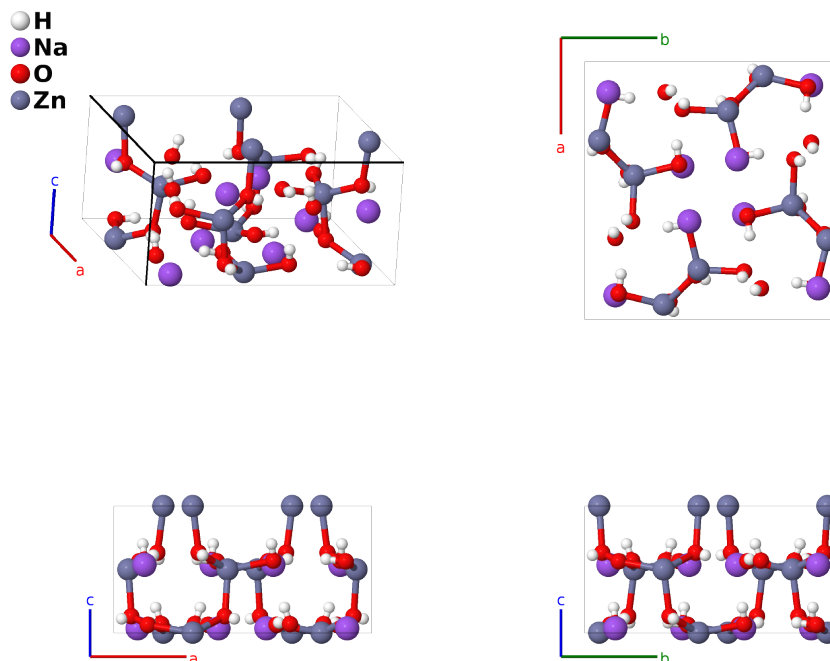
NaZn[OH]₃ Structure: A3BC3D_tP64_106_3c_c_3c_c-001

This structure originally had the label A3BC3D_tP64_106_3c_c_3c_c. Calls to that address will be redirected here.

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<https://afLOW.org/p/SP8Q>

https://afLOW.org/p/A3BC3D_tP64_106_3c_c_3c_c-001

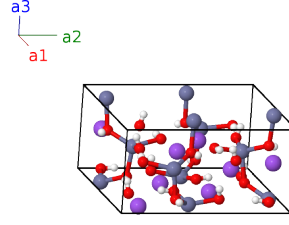


Prototype	H ₃ NaO ₃ Zn
AFLOW prototype label	A3BC3D_tP64_106_3c_c_3c_c-001
ICSD	66975
Pearson symbol	tP64
Space group number	106
Space group symbol	<i>P</i> 4 ₂ <i>bc</i>
AFLOW prototype command	<pre>afLOW --proto=A3BC3D_tP64_106_3c_c_3c_c-001 --params=a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈</pre>

- Space group *P*4₂*bc* #106 allows an arbitrary placement of the origin of the *z*-axis. Here we use this freedom to set $z_8 = 0$ for the zinc atoms.
- The O-II – H-II distance is unreasonably small (0.45Å). It is likely that there is an error in the coordinates for one of these atoms.

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8c)	H I
\mathbf{B}_2	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$-ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8c)	H I
\mathbf{B}_3	$-y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$-ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	H I
\mathbf{B}_4	$y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	H I
\mathbf{B}_5	$(x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8c)	H I
\mathbf{B}_6	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8c)	H I
\mathbf{B}_7	$-(y_1 - \frac{1}{2}) \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(y_1 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	H I
\mathbf{B}_8	$(y_1 + \frac{1}{2}) \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$a(y_1 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	H I
\mathbf{B}_9	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c)	H II
\mathbf{B}_{10}	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c)	H II
\mathbf{B}_{11}	$-y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$-ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	H II
\mathbf{B}_{12}	$y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	H II
\mathbf{B}_{13}	$(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c)	H II
\mathbf{B}_{14}	$-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c)	H II
\mathbf{B}_{15}	$-(y_2 - \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	H II
\mathbf{B}_{16}	$(y_2 + \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$a(y_2 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	H II
\mathbf{B}_{17}	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	H III
\mathbf{B}_{18}	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	H III
\mathbf{B}_{19}	$-y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	H III
\mathbf{B}_{20}	$y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	H III
\mathbf{B}_{21}	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	H III
\mathbf{B}_{22}	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	H III

$$\begin{aligned}
\mathbf{B}_{55} &= -\left(y_7 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_7 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \quad \text{O III} \\
\mathbf{B}_{56} &= \left(y_7 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \quad \text{O III} \\
\mathbf{B}_{57} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \quad \text{Zn I} \\
\mathbf{B}_{58} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \quad \text{Zn I} \\
\mathbf{B}_{59} &= -y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= -ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \quad \text{Zn I} \\
\mathbf{B}_{60} &= y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \quad \text{Zn I} \\
\mathbf{B}_{61} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \quad \text{Zn I} \\
\mathbf{B}_{62} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \quad \text{Zn I} \\
\mathbf{B}_{63} &= -\left(y_8 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_8 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \quad \text{Zn I} \\
\mathbf{B}_{64} &= \left(y_8 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_8 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \quad \text{Zn I}
\end{aligned}$$

References

- [1] R. Stahl and H. Jacobs, *Synthese und Kristallstruktur von $\text{NaZn}(\text{OH})_3 \cdot 3\text{H}_2\text{O}$ und $\text{NaZn}(\text{OH})_3$* , Z. Anorganische und Allgemeine Chemie **624**, 25–29 (1998), doi:10.1002/(SICI)1521-3749(199801)624:1<25::AID-ZAAC25>3.0.CO;2-8.

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- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.