

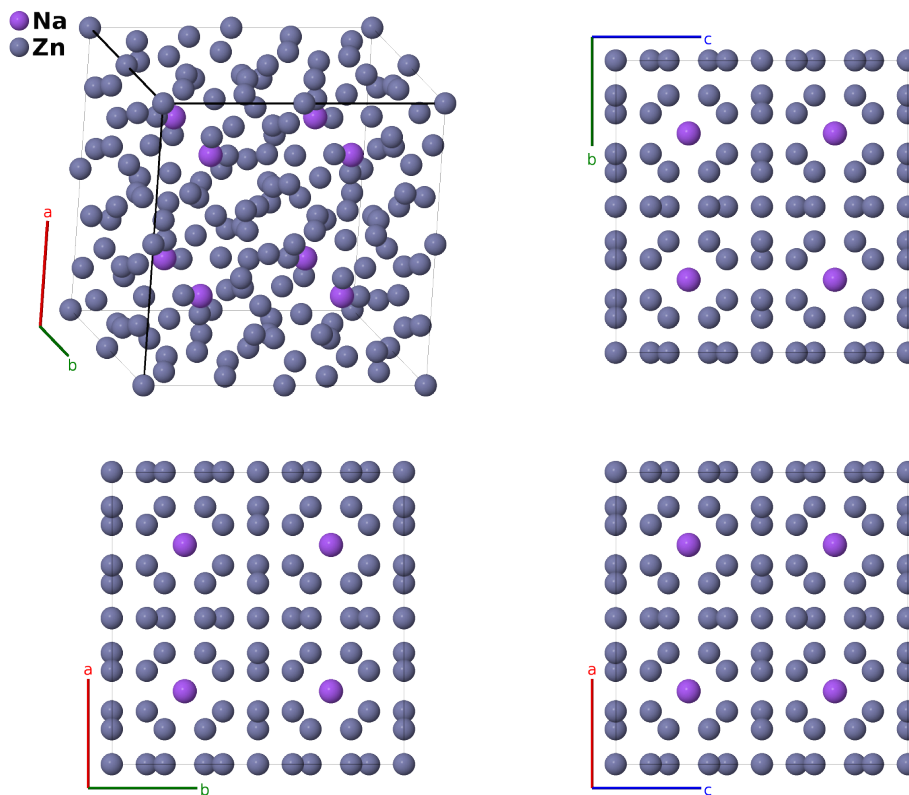
# NaZn<sub>13</sub> ( $D_{23}$ ) Structure: AB13\_cF112\_226\_a\_bi-001

This structure originally had the label AB13\_cF112.226\_a.bi. Calls to that address will be redirected here.

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

[https://afLOW.org/p/AB13\\_cF112\\_226\\_a\\_bi-001](https://afLOW.org/p/AB13_cF112_226_a_bi-001)



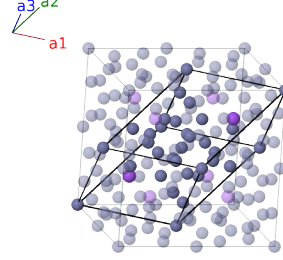
Prototype	NaZn <sub>13</sub>
AFLOW prototype label	AB13_cF112_226_a_bi-001
<i>Strukturbericht</i> designation	$D_{23}$
ICSD	105173
Pearson symbol	cF112
Space group number	226
Space group symbol	$Fm\bar{3}c$
AFLOW prototype command	<code>afLOW --proto=AB13_cF112_226_a_bi-001 --params=a, y<sub>3</sub>, z<sub>3</sub></code>

### Other compounds with this structure

AmBe<sub>13</sub>, BaCu<sub>13</sub>, BaZn<sub>13</sub>, CaBe<sub>13</sub>, CaZn<sub>13</sub>, CdZn<sub>13</sub>, CeBe<sub>13</sub>, CsCd<sub>13</sub>, DyBe<sub>13</sub>, ErBe<sub>13</sub>, EuBe<sub>13</sub>, HfBe<sub>13</sub>, KCd<sub>13</sub>, KZn<sub>13</sub>, LaBe<sub>13</sub>, LuBe<sub>13</sub>, MgBe<sub>13</sub>, NbBe<sub>13</sub>, NdBe<sub>13</sub>, PtBe<sub>13</sub>, PuBe<sub>13</sub>, RbCd<sub>13</sub>, ScBe<sub>13</sub>, SmBe<sub>13</sub>, SrBe<sub>13</sub>, SrZn<sub>13</sub>, TbBe<sub>13</sub>, ThBe<sub>13</sub>, TmBe<sub>13</sub>, UBe<sub>13</sub>, VBe<sub>13</sub>, YBe<sub>13</sub>, YbBe<sub>13</sub>, ZrBe<sub>13</sub>, CeNi<sub>8.5</sub>Si<sub>4.5</sub>, LaFe<sub>13-x-y</sub>Co<sub>y</sub>Al<sub>x</sub>, LaFe<sub>13-x-y</sub>Co<sub>y</sub>Si<sub>x</sub>, NdFe<sub>13-x-y</sub>Co<sub>y</sub>Si<sub>x</sub>

### Face-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{y} + \frac{1}{2}a \hat{z} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{x} + \frac{1}{2}a \hat{z} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{x} + \frac{1}{2}a \hat{y}\end{aligned}$$



### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{x} + \frac{1}{4}a \hat{y} + \frac{1}{4}a \hat{z}$	(8a)	Na I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{x} + \frac{3}{4}a \hat{y} + \frac{3}{4}a \hat{z}$	(8a)	Na I
$\mathbf{B}_3$	$= 0$	$=$	$0$	(8b)	Zn I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{x} + \frac{1}{2}a \hat{y} + \frac{1}{2}a \hat{z}$	(8b)	Zn I
$\mathbf{B}_5$	$= (y_3 + z_3) \mathbf{a}_1 - (y_3 - z_3) \mathbf{a}_2 + (y_3 - z_3) \mathbf{a}_3$	$=$	$ay_3 \hat{y} + az_3 \hat{z}$	(96i)	Zn II
$\mathbf{B}_6$	$= -(y_3 - z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 - (y_3 + z_3) \mathbf{a}_3$	$=$	$-ay_3 \hat{y} + az_3 \hat{z}$	(96i)	Zn II
$\mathbf{B}_7$	$= (y_3 - z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$=$	$ay_3 \hat{y} - az_3 \hat{z}$	(96i)	Zn II
$\mathbf{B}_8$	$= -(y_3 + z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3$	$=$	$-ay_3 \hat{y} - az_3 \hat{z}$	(96i)	Zn II
$\mathbf{B}_9$	$= (y_3 - z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3$	$=$	$az_3 \hat{x} + ay_3 \hat{z}$	(96i)	Zn II
$\mathbf{B}_{10}$	$= -(y_3 + z_3) \mathbf{a}_1 - (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$=$	$az_3 \hat{x} - ay_3 \hat{z}$	(96i)	Zn II
$\mathbf{B}_{11}$	$= (y_3 + z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 - (y_3 + z_3) \mathbf{a}_3$	$=$	$-az_3 \hat{x} + ay_3 \hat{z}$	(96i)	Zn II
$\mathbf{B}_{12}$	$= -(y_3 - z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 + (y_3 - z_3) \mathbf{a}_3$	$=$	$-az_3 \hat{x} - ay_3 \hat{z}$	(96i)	Zn II
$\mathbf{B}_{13}$	$= -(y_3 - z_3) \mathbf{a}_1 + (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$=$	$ay_3 \hat{x} + az_3 \hat{y}$	(96i)	Zn II
$\mathbf{B}_{14}$	$= (y_3 + z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3$	$=$	$-ay_3 \hat{x} + az_3 \hat{y}$	(96i)	Zn II
$\mathbf{B}_{15}$	$= -(y_3 + z_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 + (y_3 - z_3) \mathbf{a}_3$	$=$	$ay_3 \hat{x} - az_3 \hat{y}$	(96i)	Zn II
$\mathbf{B}_{16}$	$= (y_3 - z_3) \mathbf{a}_1 - (y_3 - z_3) \mathbf{a}_2 - (y_3 + z_3) \mathbf{a}_3$	$=$	$-ay_3 \hat{x} - az_3 \hat{y}$	(96i)	Zn II

$$\begin{aligned}
\mathbf{B}_{17} &= \begin{aligned} & -\left(y_3 + z_3 - \frac{1}{2}\right) \mathbf{a}_1 + \\ & \left(y_3 - z_3 + \frac{1}{2}\right) \mathbf{a}_2 + \\ & \left(y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_3 \end{aligned} &= & a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96i) & \text{Zn II} \\
\mathbf{B}_{18} &= \begin{aligned} & \left(y_3 - z_3 + \frac{1}{2}\right) \mathbf{a}_1 - \\ & \left(y_3 + z_3 - \frac{1}{2}\right) \mathbf{a}_2 + \\ & \left(-y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_3 \end{aligned} &= & -a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} - a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96i) & \text{Zn II} \\
\mathbf{B}_{19} &= \begin{aligned} & \left(-y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_1 + \\ & \left(y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_2 + \\ & \left(y_3 - z_3 + \frac{1}{2}\right) \mathbf{a}_3 \end{aligned} &= & a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} & (96i) & \text{Zn II} \\
\mathbf{B}_{20} &= \begin{aligned} & \left(y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_1 + \\ & \left(-y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_2 - \\ & \left(y_3 + z_3 - \frac{1}{2}\right) \mathbf{a}_3 \end{aligned} &= & -a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} & (96i) & \text{Zn II} \\
\mathbf{B}_{21} &= \begin{aligned} & \left(-y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_1 - \\ & \left(y_3 + z_3 - \frac{1}{2}\right) \mathbf{a}_2 + \\ & \left(y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_3 \end{aligned} &= & \frac{1}{2}a\hat{\mathbf{x}} + a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96i) & \text{Zn II} \\
\mathbf{B}_{22} &= \begin{aligned} & \left(y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_1 + \\ & \left(y_3 - z_3 + \frac{1}{2}\right) \mathbf{a}_2 + \\ & \left(-y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_3 \end{aligned} &= & \frac{1}{2}a\hat{\mathbf{x}} + a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{z}} & (96i) & \text{Zn II} \\
\mathbf{B}_{23} &= \begin{aligned} & -\left(y_3 + z_3 - \frac{1}{2}\right) \mathbf{a}_1 + \\ & \left(-y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_2 + \\ & \left(y_3 - z_3 + \frac{1}{2}\right) \mathbf{a}_3 \end{aligned} &= & \frac{1}{2}a\hat{\mathbf{x}} - a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96i) & \text{Zn II} \\
\mathbf{B}_{24} &= \begin{aligned} & \left(y_3 - z_3 + \frac{1}{2}\right) \mathbf{a}_1 + \\ & \left(y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_2 - \\ & \left(y_3 + z_3 - \frac{1}{2}\right) \mathbf{a}_3 \end{aligned} &= & \frac{1}{2}a\hat{\mathbf{x}} - a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{z}} & (96i) & \text{Zn II} \\
\mathbf{B}_{25} &= \begin{aligned} & \left(y_3 - z_3 + \frac{1}{2}\right) \mathbf{a}_1 + \\ & \left(-y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_2 + \\ & \left(y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_3 \end{aligned} &= & a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} & (96i) & \text{Zn II} \\
\mathbf{B}_{26} &= \begin{aligned} & -\left(y_3 + z_3 - \frac{1}{2}\right) \mathbf{a}_1 + \\ & \left(y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_2 + \\ & \left(-y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_3 \end{aligned} &= & a\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} & (96i) & \text{Zn II} \\
\mathbf{B}_{27} &= \begin{aligned} & \left(y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_1 - \\ & \left(y_3 + z_3 - \frac{1}{2}\right) \mathbf{a}_2 + \\ & \left(y_3 - z_3 + \frac{1}{2}\right) \mathbf{a}_3 \end{aligned} &= & -a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} & (96i) & \text{Zn II} \\
\mathbf{B}_{28} &= \begin{aligned} & \left(-y_3 + z_3 + \frac{1}{2}\right) \mathbf{a}_1 + \\ & \left(y_3 - z_3 + \frac{1}{2}\right) \mathbf{a}_2 - \\ & \left(y_3 + z_3 - \frac{1}{2}\right) \mathbf{a}_3 \end{aligned} &= & -a\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}} & (96i) & \text{Zn II}
\end{aligned}$$

## References

- [1] D. P. Shoemaker, R. E. Marsh, F. J. Ewing, and L. Pauling, *Interatomic distances and atomic valences in NaZn<sub>13</sub>*, *Acta Cryst.* **5**, 637–644 (1952), doi:10.1107/S0365110X52001763.