

NaZn₁₃ (*D*2₃) Structure: AB13_cF112_226_a_bi-001

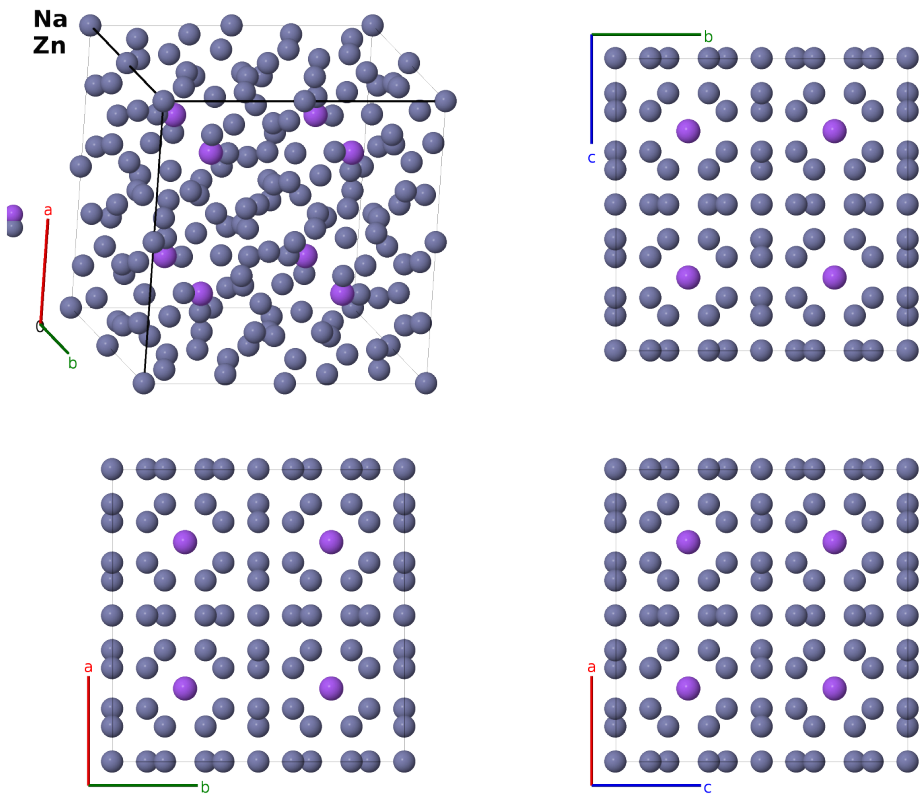
This structure previously used the label(s) **AB13_cF112_226_a_bi**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/DCLX>

https://aflow.org/prototype-encyclopedia/AB13_cF112_226_a_bi-001



Prototype	NaZn ₁₃
AFLOW prototype label	AB13_cF112_226_a_bi-001
<i>Strukturbericht</i> designation	<i>D</i> 2 ₃
ICSD	105173
CCDC	1663064
Pearson symbol	cF112
Space group number	226
Space group symbol	<i>Fm</i> $\bar{3}$ <i>c</i>

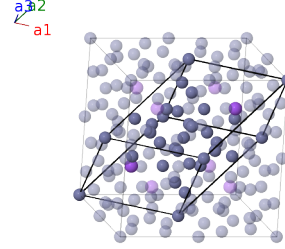
AFLOW prototype command `aflow --proto=AB13_cF112_226_a_bi-001`
 `--params=a, y3, z3`

Other compounds with this structure

AmBe₁₃, BaCu₁₃, BaZn₁₃, CaBe₁₃, CaZn₁₃, CdZn₁₃, CeBe₁₃, CsCd₁₃, DyBe₁₃, ErBe₁₃, EuBe₁₃, HfBe₁₃, KCd₁₃, KZn₁₃, LaBe₁₃, LuBe₁₃, MgBe₁₃, NbBe₁₃, NdBe₁₃, PtBe₁₃, PuBe₁₃, RbCd₁₃, ScBe₁₃, SmBe₁₃, SrBe₁₃, SrZn₁₃, TbBe₁₃, ThBe₁₃, TmBe₁₃, UBe₁₃, VBe₁₃, YBe₁₃, YbBe₁₃, ZrBe₁₃, CeNi_{8.5}Si_{4.5}, LaFe_{13-x-y}Co_yAl_x, LaFe_{13-x-y}Co_ySi_x, NdFe_{13-x-y}Co_ySi_x

Face-centered Cubic primitive vectors

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



Basis vectors

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

$$\begin{aligned}
\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{\mathbf{x}} - az_3 \hat{\mathbf{y}} &(96i) &\text{Zn II} \\
\mathbf{B}_{17} &= -\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 &= 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} &= \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 &= -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} &= \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 &= 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} &= \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 &= -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} &= \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 &= \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} &= \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 &= \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} &= -\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 &= \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} &= \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 &= \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} &= \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 &= 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} &= -\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 &= 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} &= \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 &= -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} &= \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 &= -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 NaZn₁₃*, Acta Cryst. **5**, 637–644 (1952), doi:10.1107/S0365110X52001763.

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