

Zincblende (ZnAs, *B3*) Structure: AB_cF8_216_a_c-001

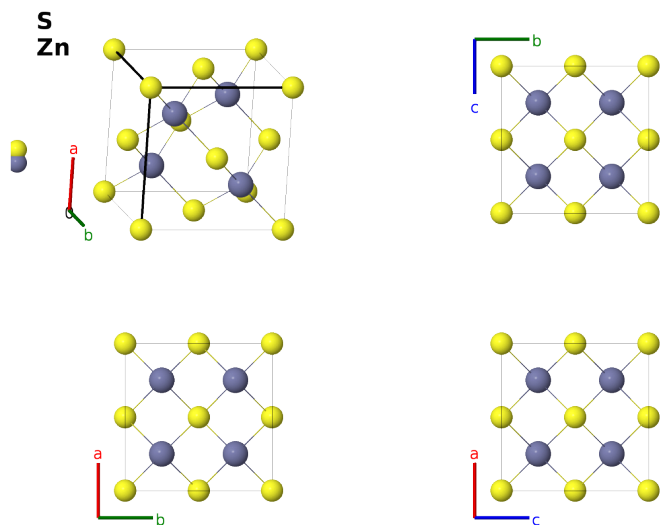
This structure previously used the label(s) **AB_cF8_216_c_a**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/TL8Z>

https://aflow.org/prototype-encyclopedia/AB_cF8_216_a_c-001



Prototype	SZn
AFLOW prototype label	AB_cF8_216_a_c-001
<i>Strukturbericht</i> designation	<i>B3</i>
Mineral name	zincblende
ICSD	651457
CCDC	1764681
Pearson symbol	cF8
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	<code>aflow --proto=AB_cF8_216_a_c-001 --params=a</code>

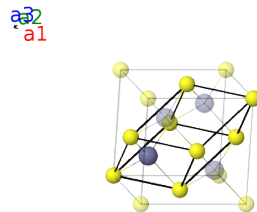
Other compounds with this structure

AgI, AlAs, AlP, AlSb, AsB, AsGa, AsIn, BN, BePo, BeS, BeSe, BeTe, β -CsSi, CdPo, CdS, CdSe, CdTe, CuI (marshite), FeN, GaP, GaSb, HgS, HgSe, HgTe, InP, InSb, β -MnS, β -MnSe, OZn, PoZn, SSn, SZn, TeZn, (Fe, Zn)S (sphalerite)

- This is the cubic analog of wurtzite ($B4$), *i.e.* the stacking of the ZnS dimers along the $\langle 111 \rangle$ direction is ABCABC ... This is also a two-component analog of diamond ($A4$), without the inversion symmetry in the middle of the bond.
- Zincblende may also be referred to as sphalerite.

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
$\mathbf{B}_1$	=	0	=	0	(4a) S I
$\mathbf{B}_2$	=	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	=	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(4c) Zn I

References

- [1] B. J. Skinner, *Unit-Cell Edges of Natural and Synthetic Sphalerites*, Am. Mineral. **46**, 1399–1411 (1961).

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

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017