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

This structure originally had the label `AB_cF8_216_c_a`. Calls to that address will be redirected here.

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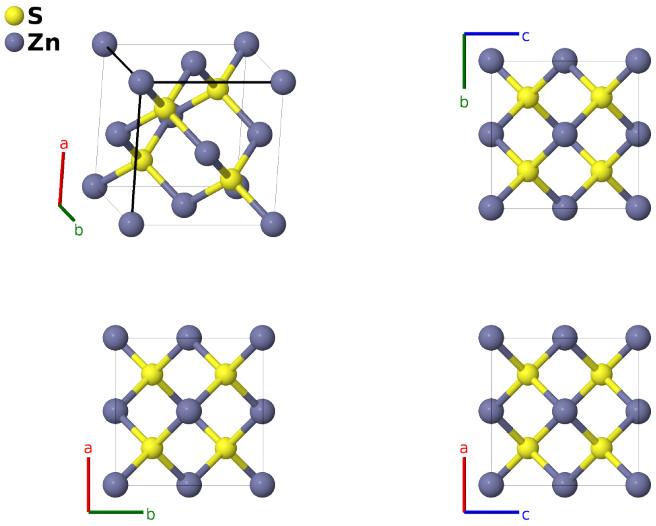
https://aflow.org/p/TL8Z

https://aflow.org/p/AB_cF8_216_a_c-001



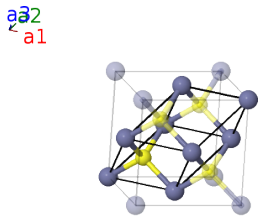
Prototype	SZn
AFLOW prototype label	AB_cF8_216_a_c-001
***Strukturbericht* designation**	$B3$
Mineral name	zincblende
ICSD	651457
Pearson symbol	cF8
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	`aflow --proto=AB_cF8_216_a_c-001 --params=`a

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 $< 111 >$ 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

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$$



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).