Wurtzite (ZnS, $B4$) Structure: AB_hP4_186_b_b-001

This structure originally had the label `AB_hP4_186_b_b`. Calls to that address will be redirected here.

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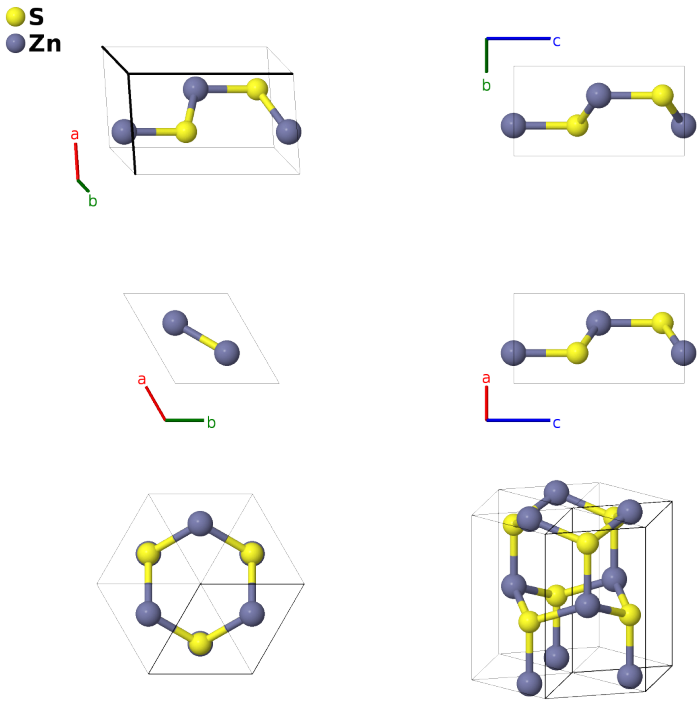
https://aflow.org/p/6CGK

https://aflow.org/p/AB_hP4_186_b_b-001



Prototype	SZn
AFLOW prototype label	AB_hP4_186_b_b-001
***Strukturbericht* designation**	$B4$
Mineral name	wurtzite
ICSD	67453
Pearson symbol	hP4
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=AB_hP4_186_b_b-001 --params=`$a, c/a, z_1, z_2$

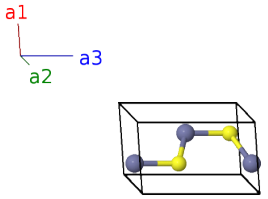
Other compounds with this structure

β-AgI, AlN, BN, BeO, CdS, CdSe, CdSe, CuH, β-CuI, GaN, InN, MgTe, γ-MnS, γ-MnSe, SiC, ZnO, ZnSe

- This is the hexagonal analog of zincblende ($B3$), *i.e.* the stacking of the ZnS dimers along the (0001) direction is ABABAB... Replacing both the Zn and S atoms by C (or Si) gives the hexagonal diamond structure. The "ideal" structure, where the nearest-neighbor environment of each atom is the same as in zincblende, is achieved when we take $c/a = \sqrt{8/3}$ and $z_2 = 1/8$. In the extreme case $z_2 = 1/2$ this structure becomes the BN (B_k) structure.
- We have arbitrarily chosen the z_2 parameter for the zinc atoms to be zero, as allowed by space group $P6_3mc$ #186.

Hexagonal primitive vectors

$$\begin{aligned} \mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}} \end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2b)	S I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	S I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2b)	Zn I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Zn I

References

[1] E. H. Kisi and M. M. Elcombe, *u parameters for the wurtzite structure of ZnS and ZnO using powder neutron diffraction*, Acta Crystallogr. Sect. C **45**, 1867–1870 (1989), doi:10.1107/S0108270189004269.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).