

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

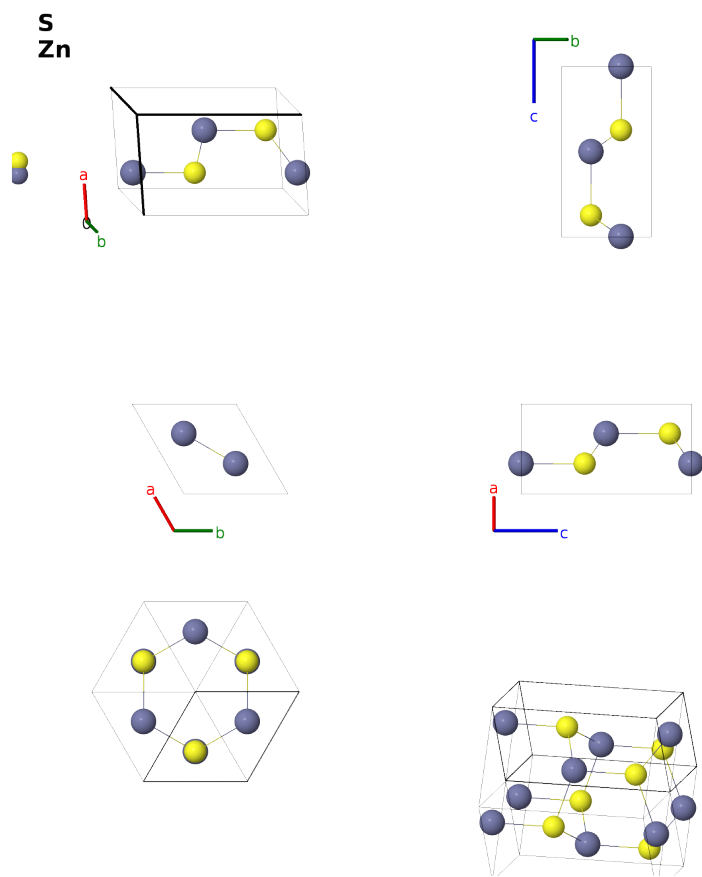
This structure previously used the label(s) **AB_hP4_186_b_b**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/6CGK>

https://aflow.org/prototype-encyclopedia/AB_hP4_186_b_b-001



Prototype	SZn
AFLOW prototype label	AB_hP4_186_b_b-001
<i>Strukturbericht</i> designation	<i>B4</i>
Mineral name	wurtzite
ICSD	67453
CCDC	1629447
Pearson symbol	hP4

Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	<code>aflow --proto=AB_hP4_186_b_b-001</code> <code>--params=a, c/a, z₁, z₂</code>

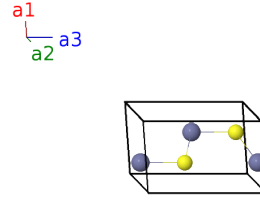
Other compounds with this structure

β -AgI, AlN, BN, BeO, CdS, 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.
- Space group $P6_3$ #186 is polar, so there is no fixed origin for the z axis. We have arbitrarily chosen the z_2 parameter for the zinc atoms to be zero.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



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
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(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).

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