Bohdanowiczite ($AgBiSe_2$) Structure: ABC2_hP12_164_ad_bd_c2d-001

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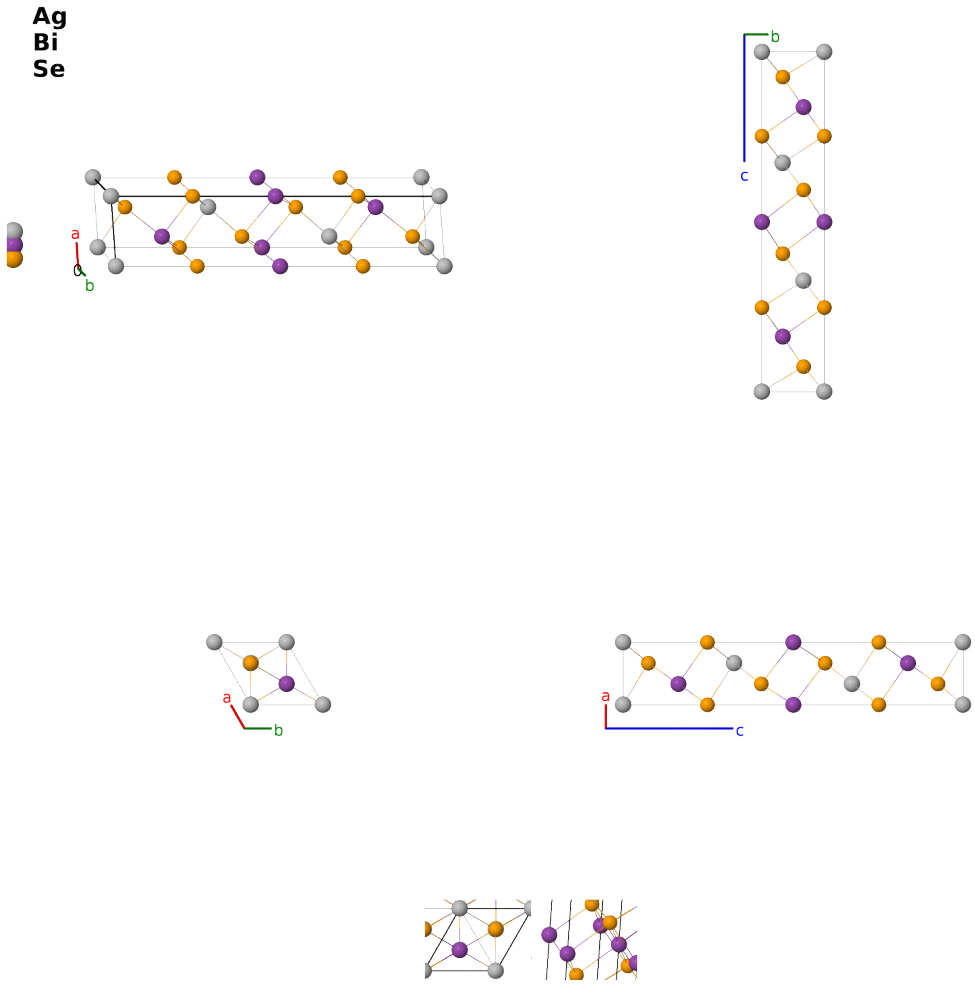
https://aflow.org/prototype-encyclopedia/1TV2

https://aflow.org/prototype-encyclopedia/ABC2_hP12_164_ad_bd_c2d-001



Prototype	$AgBiSe_2$
AFLOW prototype label	ABC2_hP12_164_ad_bd_c2d-001
Mineral name	bohdanowiczite
ICSD	26519
CCDC	1601917
Pearson symbol	hP12
Space group number	164

Space group symbol $P\bar{3}m1$

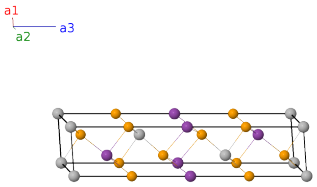
AFLOW prototype command `aflow --proto=ABC2_hP12_164_ad_bd_c2d-001 --params=`$a, c/a, z_3, z_4, z_5, z_6, z_7$

Other compounds with this structure
$AgBiS_2$, $AgBiTe_2$

- This is the ground state of $AgBiSe_2$. According to the phase diagram in (Villars, 2018) this transforms into the rhombohedral α-$NaFeO_2$ structure at 365°C. (Geller, 1959) agree that this is a high-temperature state, but say that it exists between 120°C and 287°C. Above this temperature they say that $AgBiSe_2$ transforms into the NaCl ($B1$) structure, with silver and bismuth randomly placed on the "Na" site and selenium on the "Cl" site.
- (Geller, 1959) note that the trigonal ground state and the rhombohedral high-temperature state are very close together, with only small changes in the atomic coordinates needed to transform one into the other.
- The $MnBi_4Te_7$ structure occupies the same Wyckoff positions with a different stoichiometry. The ICSD lists $AgBiSe_2$ as the prototype for all of these structures, but we have split them to reflect the chemistry of the structures.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Ag I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Bi I
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2c)	Se I
$\mathbf{B_4}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(2c)	Se I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2d)	Ag II
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2d)	Ag II
$\mathbf{B_7}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(2d)	Bi II
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(2d)	Bi II
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(2d)	Se II
$\mathbf{B_{10}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(2d)	Se II
$\mathbf{B_{11}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(2d)	Se III
$\mathbf{B_{12}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(2d)	Se III

References

[1] S. Geller and J. H. Wernick, *Ternary semiconducting compounds with sodium chloride-like structure: $AgSbSe_2$, $AgSbTe_2$, $AgBiS_2$, $AgBiSe_2$*, Acta Cryst. **12**, 46–54 (1959), doi:10.1107/S0365110X59000135.

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[1] P. Villars, H. Okamoto, and K. Cenzual, eds., *ASM Alloy Phase Diagram Database* (ASM International, 2018), chap. Silver-Bismuth-Selenium Ternary, Vertical Section (1966 Hirai T.). Copyright ©2006-2018 ASM International.

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