

α -Naumannite (Ag_2Se) Structure: A2B_oP12_17_abe_e-001

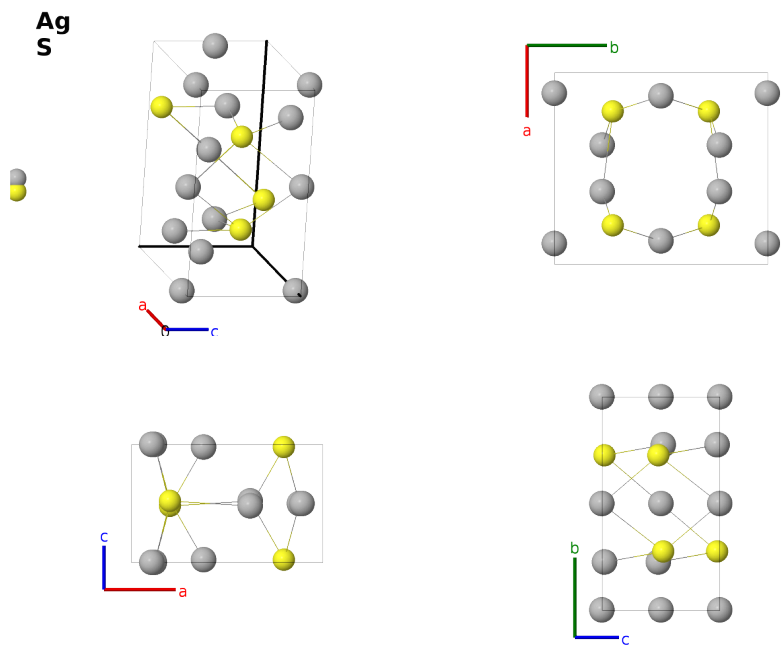
This structure previously used the label(s) **A2B_oP12_17_abe_e**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/G353>

https://aflow.org/prototype-encyclopedia/A2B_oP12_17_abe_e-001

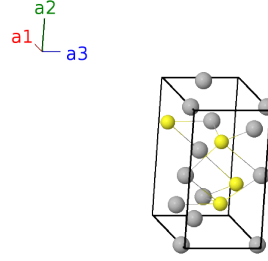


Prototype	Ag_2Se
AFLOW prototype label	A2B_oP12_17_abe_e-001
Mineral name	naumannite
ICSD	43242
CCDC	1612764
Pearson symbol	oP12
Space group number	17
Space group symbol	$P222_1$
AFLOW prototype command	<code>aflow --proto=A2B_oP12_17_abe_e-001</code> <code>--params=$a, b/a, c/a, x_1, x_2, x_3, y_3, z_3, x_4, y_4, z_4$</code>

- The low temperature form of nauminnite is stable below 133°C (Wiegers, 1971). This structure (Pinsker, 1965) disagrees with that found by that found by (Wiegers, 1971).

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1$	$=$	$ax_1 \hat{\mathbf{x}}$	(2a)	Ag I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2a)	Ag I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$	(2b)	Ag II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(2b)	Ag II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4e)	Ag III
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Ag III
$\mathbf{B}_7$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Ag III
$\mathbf{B}_8$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4e)	Ag III
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_{11}$	$= -x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B}_{12}$	$= x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4e)	S I

References

- [1] Z. G. Pinsker, C. Ching-liang, R. M. Imamov, and E. L. Lapidus, *Determination of the crystal structure of the low-temperature phase α -Ag₂Se*, Sov. Phys. Crystallogr. **10**, 225–231 (1965).
- [2] G. A. Wiegers, *The Crystal Structure of the Low-Temperature Form of Silver Selenide*, Am. Mineral. **56**, 1882–1888 (1971).

Found in

- [1] P. Villars, *FeS Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database).

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