α-Naumannite (Ag_2Se) Structure: A2B_oP12_17_abe_e-001

This structure originally had the label `A2B_oP12_17_abe_e`. Calls to that address will be redirected here.

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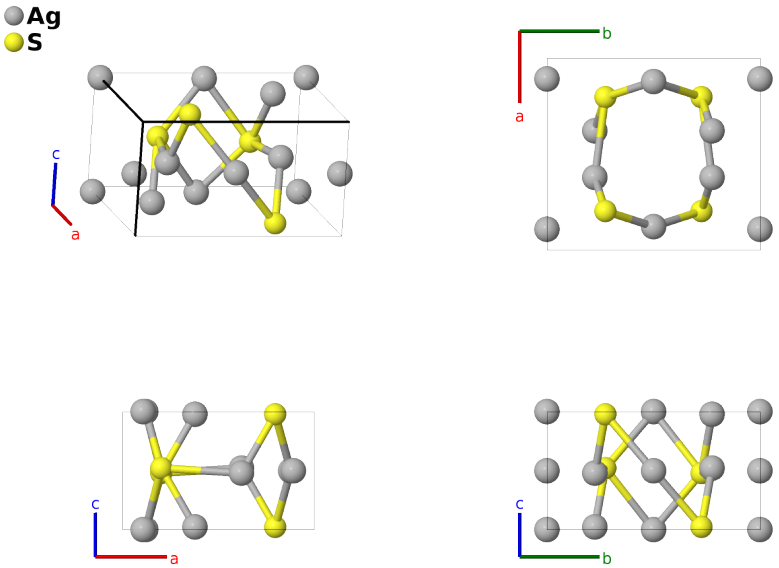
https://aflow.org/p/G353

https://aflow.org/p/A2B_oP12_17_abe_e-001

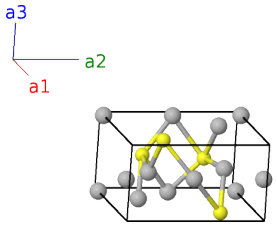


Prototype	Ag_2Se
AFLOW prototype label	A2B_oP12_17_abe_e-001
Mineral name	naumannite
ICSD	43242
Pearson symbol	oP12
Space group number	17
Space group symbol	$P222_1$
AFLOW prototype command	`aflow --proto=A2B_oP12_17_abe_e-001 --params=`$a, b/a, c/a, x_1, x_2, x_3, y_3, z_3, x_4, y_4, z_4$

- 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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Ag III
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	S I
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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-Ag_2Se*, 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).