

Cs₂Se Structure:

A2B_oF24_43_b_a-001

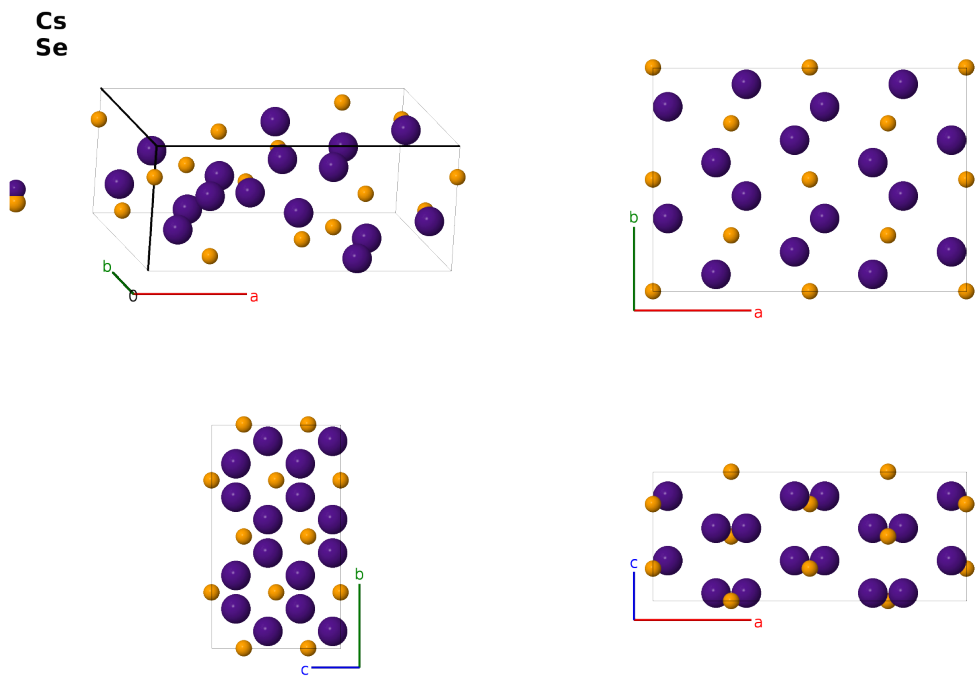
This structure previously used the label(s) **A2B_oF24_43_b_a**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/DUC7>

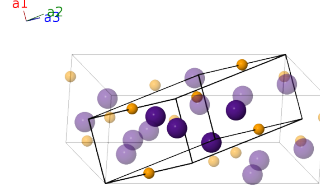
https://aflow.org/prototype-encyclopedia/A2B_oF24_43_b_a-001



Prototype	Cs ₂ Se
AFLOW prototype label	A2B_oF24_43_b_a-001
ICSD	41687
CCDC	1611448
Pearson symbol	oF24
Space group number	43
Space group symbol	<i>Fdd</i> 2
AFLOW prototype command	<code>aflow --proto=A2B_oF24_43_b_a-001</code> <code>--params=a, b/a, c/a, z₁, x₂, y₂, z₂</code>

Face-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(8a)	Se I
$\mathbf{B}_2$	$= \left(z_1 + \frac{1}{4}\right) \mathbf{a}_1 + \left(z_1 + \frac{1}{4}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(8a)	Se I
$\mathbf{B}_3$	$= (-x_2 + y_2 + z_2) \mathbf{a}_1 + (x_2 - y_2 + z_2) \mathbf{a}_2 + (x_2 + y_2 - z_2) \mathbf{a}_3$	$=$	$ax_2\hat{\mathbf{x}} + by_2\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(16b)	Cs I
$\mathbf{B}_4$	$= (x_2 - y_2 + z_2) \mathbf{a}_1 + (-x_2 + y_2 + z_2) \mathbf{a}_2 - (x_2 + y_2 + z_2) \mathbf{a}_3$	$=$	$-ax_2\hat{\mathbf{x}} - by_2\hat{\mathbf{y}} + cz_2\hat{\mathbf{z}}$	(16b)	Cs I
$\mathbf{B}_5$	$= -\left(x_2 + y_2 - z_2 - \frac{1}{4}\right) \mathbf{a}_1 + \left(x_2 + y_2 + z_2 + \frac{1}{4}\right) \mathbf{a}_2 + \left(x_2 - y_2 - z_2 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{4}\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Cs I
$\mathbf{B}_6$	$= \left(x_2 + y_2 + z_2 + \frac{1}{4}\right) \mathbf{a}_1 - \left(x_2 + y_2 - z_2 - \frac{1}{4}\right) \mathbf{a}_2 - \left(x_2 - y_2 + z_2 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{4}\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Cs I

References

- [1] P. Böttcher, *Zur kenntnis von Cs₂Se*, J. Less-Common Met. **76**, 271–277 (1980), doi:10.1016/0022-5088(80)90029-6.

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