Cs_2Se Structure: A2B_oF24_43_b_a-001

This structure originally had the label `A2B_oF24_43_b_a`. Calls to that address will be redirected here.

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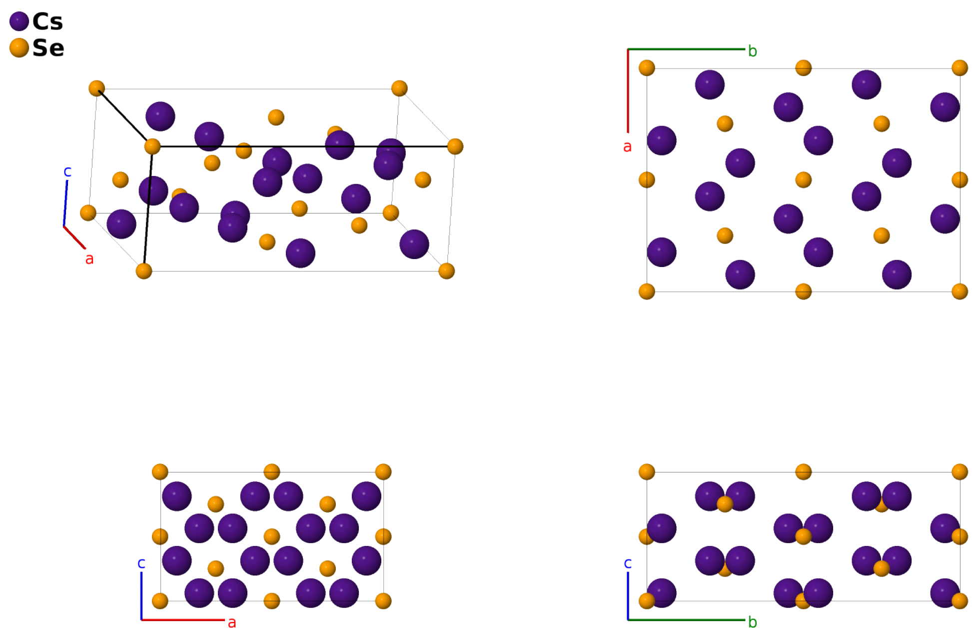
https://aflow.org/p/DUC7

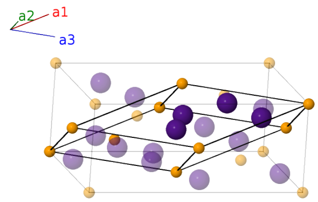
https://aflow.org/p/A2B_oF24_43_b_a-001



Prototype	Cs_2Se
AFLOW prototype label	A2B_oF24_43_b_a-001
ICSD	41687
Pearson symbol	oF24
Space group number	43
Space group symbol	$Fdd2$
AFLOW prototype command	`aflow --proto=A2B_oF24_43_b_a-001` `--params=`$a, b/a, c/a, z_1, x_2, y_2, z_2$

Face-centered Orthorhombic primitive vectors

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



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
$\mathbf{B_3}$	=	$\left(-x_2 + y_2 + z_2\right)\,\mathbf{a}_1 + \left(x_2 - y_2 + z_2\right)\,\mathbf{a}_2 + \left(x_2 + y_2 - z_2\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(16b)	Cs I
$\mathbf{B_4}$	=	$\left(x_2 - y_2 + z_2\right)\,\mathbf{a}_1 + \left(-x_2 + y_2 + z_2\right)\,\mathbf{a}_2 - \left(x_2 + y_2 + z_2\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(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 Cs_2Se*, J. Less-Common Met. **76**, 271–277 (1980), doi:10.1016/0022-5088(80)90029-6.