Ta_2Se_8I Structure: AB8C2_tI44_97_e_2k_cd-001

This structure previously used the label(s) `AB8C2_tI44_97_e_2k_cd`. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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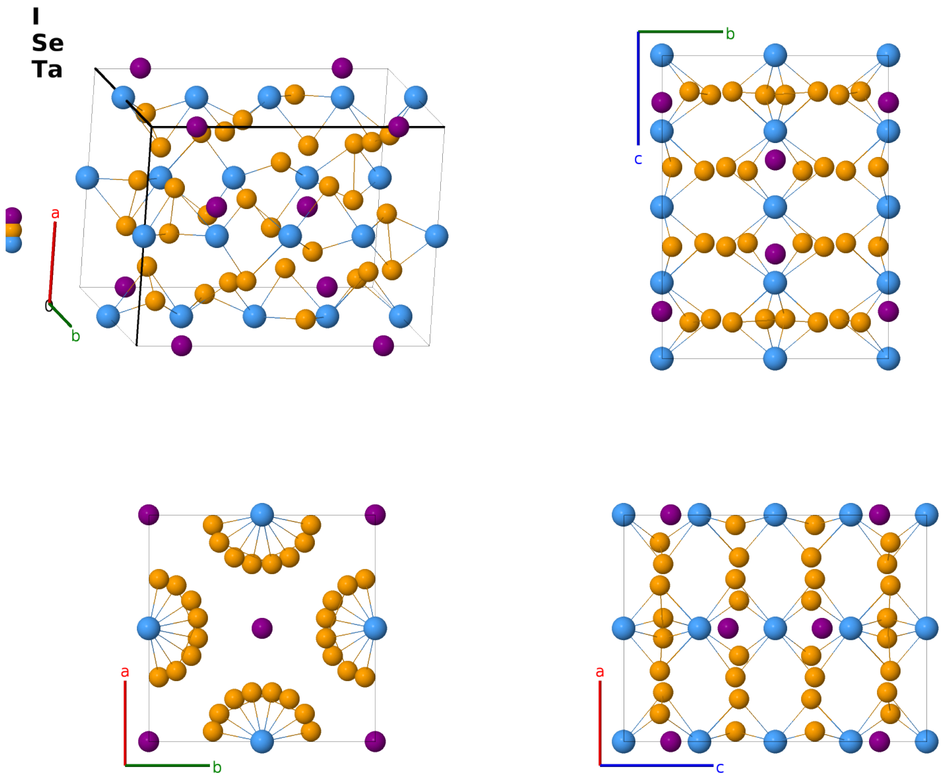
https://aflow.org/prototype-encyclopedia/4HFE

https://aflow.org/prototype-encyclopedia/AB8C2_tI44_97_e_2k_cd-001

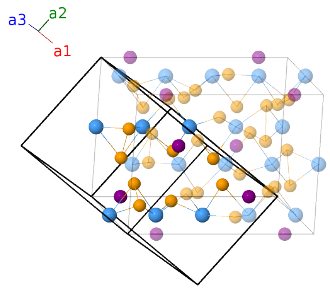


Prototype	ISe_8Ta_2
AFLOW prototype label	AB8C2_tI44_97_e_2k_cd-001
ICSD	35190
CCDC	1607337
Pearson symbol	tI44
Space group number	97
Space group symbol	$I422$
AFLOW prototype command	`aflow --proto=AB8C2_tI44_97_e_2k_cd-001` `--params=`$a, c/a, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

- The ICSD entry is from (Greissier, 1982).

Body-centered Tetragonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\mathbf{\hat{x}} + \tfrac{1}{2}a\,\mathbf{\hat{y}} + \tfrac{1}{2}c\,\mathbf{\hat{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} - \tfrac{1}{2}a\,\mathbf{\hat{y}} + \tfrac{1}{2}c\,\mathbf{\hat{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} + \tfrac{1}{2}a\,\mathbf{\hat{y}} - \tfrac{1}{2}c\,\mathbf{\hat{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{y}}$	(4c)	Ta I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}}$	(4c)	Ta I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{y}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(4d)	Ta II
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{4}c\,\mathbf{\hat{z}}$	(4d)	Ta II
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\mathbf{\hat{z}}$	(4e)	I I
$\mathbf{B_6}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\mathbf{\hat{z}}$	(4e)	I I
$\mathbf{B_7}$	=	$(y_4+z_4)\,\mathbf{a}_1 + (x_4+z_4)\,\mathbf{a}_2 + (x_4+y_4)\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} + ay_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(16k)	Se I
$\mathbf{B_8}$	=	$-(y_4-z_4)\,\mathbf{a}_1 - (x_4-z_4)\,\mathbf{a}_2 - (x_4+y_4)\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} - ay_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(16k)	Se I
$\mathbf{B_9}$	=	$(x_4+z_4)\,\mathbf{a}_1 - (y_4-z_4)\,\mathbf{a}_2 + (x_4-y_4)\,\mathbf{a}_3$	=	$-ay_4\,\mathbf{\hat{x}} + ax_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(16k)	Se I
$\mathbf{B_{10}}$	=	$-(x_4-z_4)\,\mathbf{a}_1 + (y_4+z_4)\,\mathbf{a}_2 - (x_4-y_4)\,\mathbf{a}_3$	=	$ay_4\,\mathbf{\hat{x}} - ax_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(16k)	Se I
$\mathbf{B_{11}}$	=	$(y_4-z_4)\,\mathbf{a}_1 - (x_4+z_4)\,\mathbf{a}_2 - (x_4-y_4)\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} + ay_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(16k)	Se I
$\mathbf{B_{12}}$	=	$-(y_4+z_4)\,\mathbf{a}_1 + (x_4-z_4)\,\mathbf{a}_2 + (x_4-y_4)\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} - ay_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(16k)	Se I
$\mathbf{B_{13}}$	=	$(x_4-z_4)\,\mathbf{a}_1 + (y_4-z_4)\,\mathbf{a}_2 + (x_4+y_4)\,\mathbf{a}_3$	=	$ay_4\,\mathbf{\hat{x}} + ax_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(16k)	Se I
$\mathbf{B_{14}}$	=	$-(x_4+z_4)\,\mathbf{a}_1 - (y_4+z_4)\,\mathbf{a}_2 - (x_4+y_4)\,\mathbf{a}_3$	=	$-ay_4\,\mathbf{\hat{x}} - ax_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(16k)	Se I
$\mathbf{B_{15}}$	=	$(y_5+z_5)\,\mathbf{a}_1 + (x_5+z_5)\,\mathbf{a}_2 + (x_5+y_5)\,\mathbf{a}_3$	=	$ax_5\,\mathbf{\hat{x}} + ay_5\,\mathbf{\hat{y}} + cz_5\,\mathbf{\hat{z}}$	(16k)	Se II
$\mathbf{B_{16}}$	=	$-(y_5-z_5)\,\mathbf{a}_1 - (x_5-z_5)\,\mathbf{a}_2 - (x_5+y_5)\,\mathbf{a}_3$	=	$-ax_5\,\mathbf{\hat{x}} - ay_5\,\mathbf{\hat{y}} + cz_5\,\mathbf{\hat{z}}$	(16k)	Se II
$\mathbf{B_{17}}$	=	$(x_5+z_5)\,\mathbf{a}_1 - (y_5-z_5)\,\mathbf{a}_2 + (x_5-y_5)\,\mathbf{a}_3$	=	$-ay_5\,\mathbf{\hat{x}} + ax_5\,\mathbf{\hat{y}} + cz_5\,\mathbf{\hat{z}}$	(16k)	Se II

$\mathbf{B_{18}}$	$=$	$-(x_5 - z_5)\,\mathbf{a}_1 + (y_5 + z_5)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	$=$	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16k)	Se II
$\mathbf{B_{19}}$	$=$	$(y_5 - z_5)\,\mathbf{a}_1 - (x_5 + z_5)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16k)	Se II
$\mathbf{B_{20}}$	$=$	$-(y_5 + z_5)\,\mathbf{a}_1 + (x_5 - z_5)\,\mathbf{a}_2 + (x_5 - y_5)\,\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16k)	Se II
$\mathbf{B_{21}}$	$=$	$(x_5 - z_5)\,\mathbf{a}_1 + (y_5 - z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	$=$	$ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16k)	Se II
$\mathbf{B_{22}}$	$=$	$-(x_5 + z_5)\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	$=$	$-ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(16k)	Se II

References

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First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043