Ta_2Se_8I Structure: AB8C2_tI44_97_e_2k_cd-001

This structure originally had the label `AB8C2_tI44_97_e_2k_cd`. Calls to that address will be redirected here.

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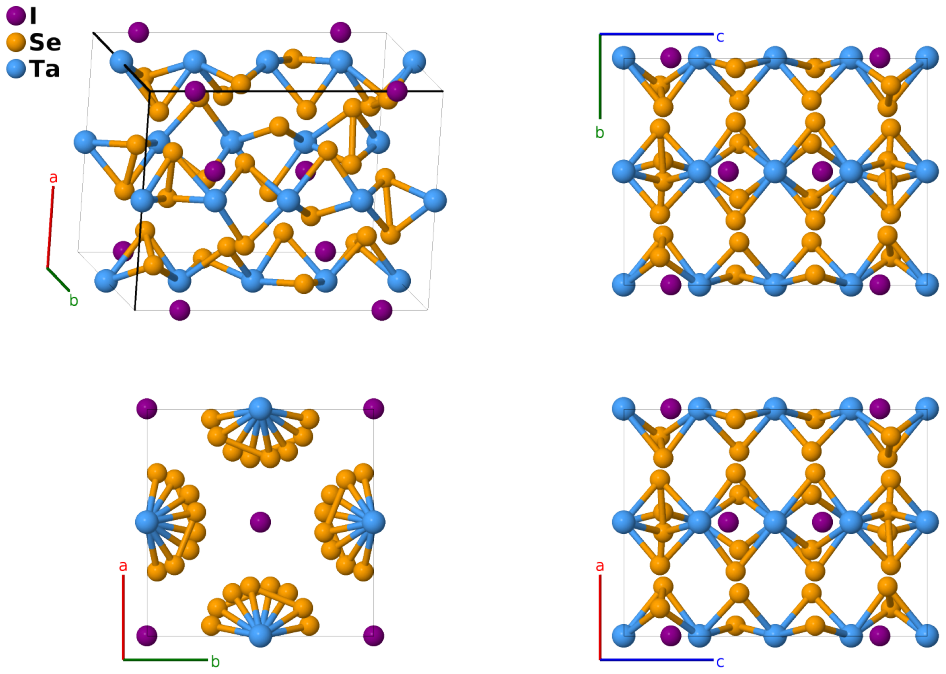
https://aflow.org/p/4HFE

https://aflow.org/p/AB8C2_tI44_97_e_2k_cd-001

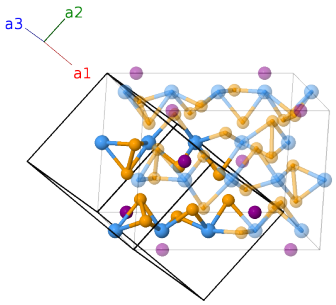


Prototype	ISe_8Ta_2
AFLOW prototype label	AB8C2_tI44_97_e_2k_cd-001
ICSD	35190
Pearson symbol	tI44
Space group number	97
Space group symbol	$I422$
AFLOW prototype command	`aflow --proto=AB8C2_tI44_97_e_2k_cd-001 --params=`$a, c/a, z_3, x_4, y_4, z_4, x_5, y_5, z_5$

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

Body-centered Tetragonal primitive vectors

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



Basis vectors

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

[1] P. Gressier, A. Meerschaut, L. Guemas, J. Rouxel, and P. Monceau, *Characterization of the new series of quasi one-dimensional compounds$(MX_4)_n Y$ (M = Nb, Ta; X =S, Se; Y =Br, I)*, J. Solid State Chem. **51**, 141–151 (1984), doi:10.1016/0022-4596(84)90327-X.

[2] P. Gressier, L. Guemas, and A. Meerschaut, *Preparation and structure of ditantalum iodide octaselenide, Ta_2ISe_8*, Acta Crystallogr. Sect. B **38**, 2877–2879 (1982), doi:10.1107/S0567740882010176.

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[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.