Ta_3S_2 Structure: A2B3_oC40_39_2d_2c2d-001

This structure originally had the label `A2B3_oC40_39_2d_2c2d`. Calls to that address will be redirected here.

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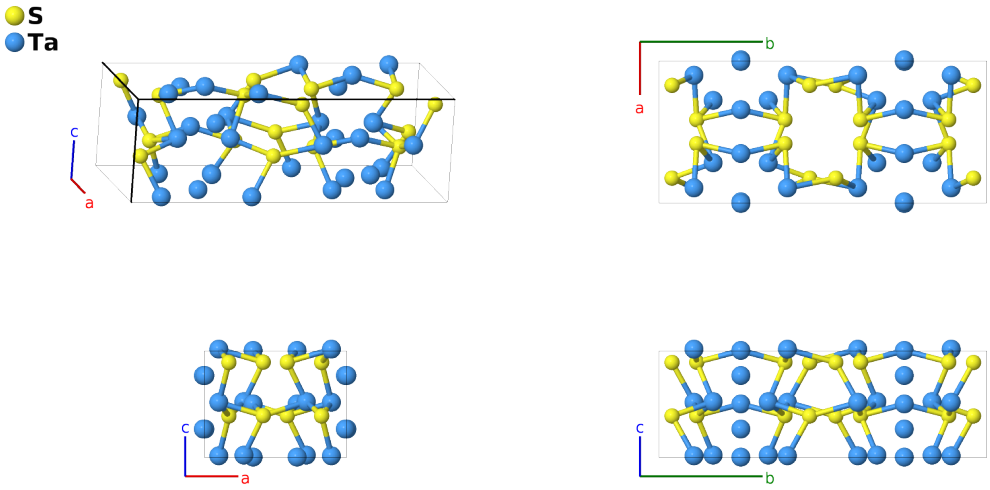
https://aflow.org/p/4YG0

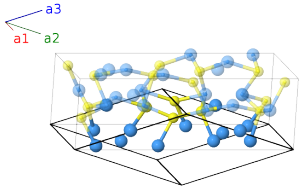
https://aflow.org/p/A2B3_oC40_39_2d_2c2d-001



Prototype	S_2Ta_3
AFLOW prototype label	A2B3_oC40_39_2d_2c2d-001
ICSD	71143
Pearson symbol	oC40
Space group number	39
Space group symbol	$Aem2$
AFLOW prototype command	`aflow --proto=A2B3_oC40_39_2d_2c2d-001 --params=`$a, b/a, c/a, x_1, z_1, x_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 - \left(z_1 - \frac{1}{4}\right)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Ta I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - \left(z_1 - \frac{3}{4}\right)\,\mathbf{a}_2 + \left(z_1 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Ta I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 - \left(z_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Ta II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - \left(z_2 - \frac{3}{4}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Ta II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 + (y_3 + z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 - (y_3 - z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - \left(y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8d)	S I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 + (y_4 + z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	S II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 - (y_4 - z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	S II
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1 - \left(y_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	S II
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8d)	S II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 + (y_5 - z_5)\,\mathbf{a}_2 + (y_5 + z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Ta III
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 - (y_5 - z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Ta III
$\mathbf{B_{15}}$	=	$x_5\,\mathbf{a}_1 - \left(y_5 + z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Ta III
$\mathbf{B_{16}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5 - z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8d)	Ta III
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1 + (y_6 - z_6)\,\mathbf{a}_2 + (y_6 + z_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	Ta IV
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1 - (y_6 + z_6)\,\mathbf{a}_2 - (y_6 - z_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	Ta IV
$\mathbf{B_{19}}$	=	$x_6\,\mathbf{a}_1 - \left(y_6 + z_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	Ta IV
$\mathbf{B_{20}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6 - z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(y_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	Ta IV

References

[1] S. J. Kim, K. S. Nanjundaswamy, and T. Hughbanks, *Single-crystal structure of tantalum sulfide (Ta_3S_2). Structure and bonding in the Ta_6S_n (n = 1,3,4,5?) pentagonal-antiprismatic chain compounds*, Inorg. Chem. **30**, 159–164 (1991), doi:10.1021/ic00002a004.

Found in

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