Ta$_2$S Structure: AB2_oP36_57_ce_2d2e-001
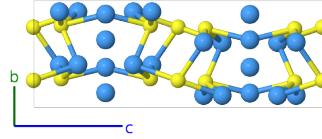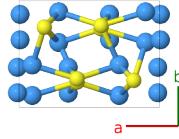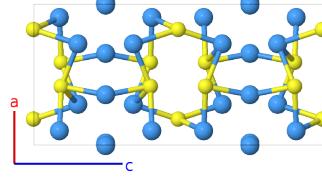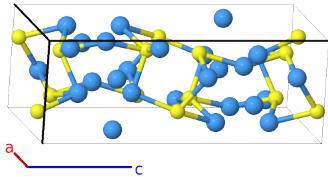
Prototype	STa$_2$
AFLOW prototype label	AB2_oP36_57_ce_2d2e-001
ICSD	26184
Pearson symbol	oP36
Space group number	57
Space group symbol	$Pbcm$
AFLOW prototype command	aflow --proto=AB2_oP36_57_ce_2d2e-001
	--params=$a, b/a, c/a, x_1, x_2, y_2, x_3, y_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- We use the Cu Kα data from (Franzen, 1969).

Simple Orthorhombic primitive vectors

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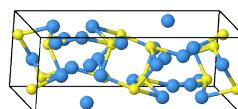$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	$=$	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}}$	(4c)	S I
$\mathbf{B_2}$	$=$	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	$=$	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_3}$	$=$	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	$=$	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}}$	(4c)	S I
$\mathbf{B_4}$	$=$	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	$=$	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4c)	S I
$\mathbf{B_5}$	$=$	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Ta I
$\mathbf{B_6}$	$=$	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	Ta I
$\mathbf{B_7}$	$=$	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-ax_2\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Ta I
$\mathbf{B_8}$	$=$	$x_2\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$ax_2\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	Ta I
$\mathbf{B_9}$	$=$	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Ta II
$\mathbf{B_{10}}$	$=$	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	Ta II
$\mathbf{B_{11}}$	$=$	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	$=$	$-ax_3\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Ta II
$\mathbf{B_{12}}$	$=$	$x_3\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	$=$	$ax_3\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	Ta II
$\mathbf{B_{13}}$	$=$	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8e)	S II
$\mathbf{B_{14}}$	$=$	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	S II
$\mathbf{B_{15}}$	$=$	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	S II
$\mathbf{B_{16}}$	$=$	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\mathbf{a}_2 - z_4\,\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8e)	S II
$\mathbf{B_{17}}$	$=$	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8e)	S II
$\mathbf{B_{18}}$	$=$	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	S II
$\mathbf{B_{19}}$	$=$	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	S II
$\mathbf{B_{20}}$	$=$	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8e)	S II
$\mathbf{B_{21}}$	$=$	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8e)	Ta III
$\mathbf{B_{22}}$	$=$	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	Ta III
$\mathbf{B_{23}}$	$=$	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	Ta III
$\mathbf{B_{24}}$	$=$	$x_5\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\mathbf{a}_2 - z_5\,\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8e)	Ta III
$\mathbf{B_{25}}$	$=$	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8e)	Ta III
$\mathbf{B_{26}}$	$=$	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	Ta III
$\mathbf{B_{27}}$	$=$	$x_5\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	Ta III
$\mathbf{B_{28}}$	$=$	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\mathbf{a}_2 + z_5\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8e)	Ta III
$\mathbf{B_{29}}$	$=$	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	$=$	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8e)	Ta IV
$\mathbf{B_{30}}$	$=$	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	Ta IV
$\mathbf{B_{31}}$	$=$	$-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	Ta IV
$\mathbf{B_{32}}$	$=$	$x_6\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\mathbf{a}_2 - z_6\,\mathbf{a}_3$	$=$	$ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8e)	Ta IV
$\mathbf{B_{33}}$	$=$	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8e)	Ta IV
$\mathbf{B_{34}}$	$=$	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	Ta IV
$\mathbf{B_{35}}$	$=$	$x_6\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\hat{\mathbf{z}}$	(8e)	Ta IV
$\mathbf{B_{36}}$	$=$	$-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\mathbf{a}_2 + z_6\,\mathbf{a}_3$	$=$	$-ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8e)	Ta IV

References

[1] H. F. Franzen and J. G. Smeggil, *The Crystal Structure of Ta$_2$S*, Acta Crystallogr. Sect. B **25**, 1736–1741 (1969), doi:10.1107/S0567740869004675.