

Ta₂S Structure:

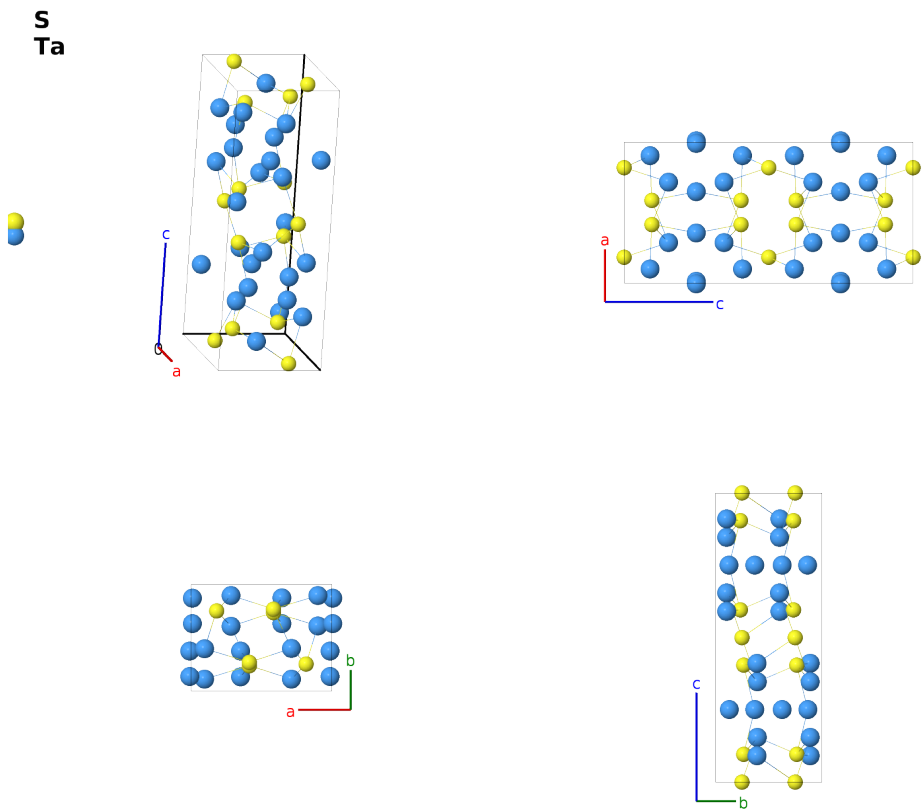
AB2_oP36_57_ce_2d2e-001

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- 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.

<https://aflow.org/prototype-encyclopedia/4L1U>

https://aflow.org/prototype-encyclopedia/AB2_oP36_57_ce_2d2e-001



Prototype	STa ₂
AFLOW prototype label	AB2_oP36_57_ce_2d2e-001
ICSD	26184
CCDC	1601617
Pearson symbol	oP36
Space group number	57
Space group symbol	<i>Pbcm</i>
AFLOW prototype command	<code>aflow --proto=AB2_oP36_57_ce_2d2e-001 --params=a,b/a,c/a,x₁,x₂,y₂,x₃,y₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆</code>

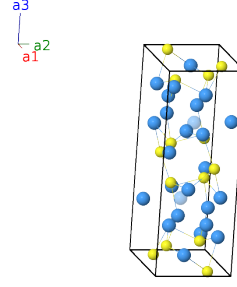
- We use the Cu K α data from (Franzen, 1969).

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
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	Ta I
$\mathbf{B}_8$	$= x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4d)	Ta II
$\mathbf{B}_{12}$	$= x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	S II
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	S II
$\mathbf{B}_{16}$	$= x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{18}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	S II
$\mathbf{B}_{19}$	$= x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	S II
$\mathbf{B}_{20}$	$= -x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(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
$\mathbf{B}_{22}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Ta III
$\mathbf{B}_{23}$	$= -x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(8e)	Ta III
$\mathbf{B}_{24}$	$= x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(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

$$\begin{aligned}
\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) &\text{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) &\text{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) &\text{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) &\text{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) &\text{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) &\text{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) &\text{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) &\text{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) &\text{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) &\text{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) &\text{Ta IV}
\end{aligned}$$

References

- [1] H. F. Franzen and J. G. Smeggil, *The Crystal Structure of Ta₂S*, Acta Crystallogr. Sect. B **25**, 1736–1741 (1969), doi:10.1107/S0567740869004675.

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